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ATMOSPHERIC DISPERSION OF HYPERGOLIC LIQUID ROCKET FUELS, (VOLUME I OF II)

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19. ABSTRACT (Continue on reverse if necessary and identify by block number) Titan II weapons systems are charged with hypergolic liquid rocket propellants (hydrazine fuel and nitrogen tetroxide oxidizer). These same propellants are used in support of other systems, including the MX missile and the space shuttle. This effort was designed to characterize the interactions of hypergolic liquid rocket propellants and to provide information pertinent to the development of a model to describe the transport and diffusion of airborne combustion products and unreacted vapors from an accident involving these propellants. This report is prepared in two volumes. Volume I addresses the reactions between nitrogen tetroxide and hydrazine, including the reaction products and the heat released. This information was used to determine the combustion time and the height of the resulting fireball before it cools and disperses with the air. Volume II discusses the chemical and physical interactions of the combustion products with air, and the dispersion of these products in the environment.												
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PREFACE

This final report, published in two volumes, was prepared by Martin Marietta Aerospace, P.O. Box 179, Denver, Colorado 80201, under Contract F42600-81-D-1379 for the Air Force Engineering and Services Center, Engineering and Services Laboratory, Tyndall Air Force Base, Florida 32403. Efforts documented in this report were performed between June 1982 and December 1983. Major Gary Worley and 2Lt Glenn Seitchek were the AFESC/RDVS project officers.

This report has been reviewed by the Public Affairs Office (PA), and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nationals.

This report has been reviewed and is approved for publication.

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SECTION I

INTRODUCTION

The Titan II Weapons System is deployed at sites in Arizona, Arkansas, and Kansas. Although these sites were rural when initially deployed in the 1960s, land development and population expansion has gradually encroached upon many of the current sites. Because the Titan II Weapons System is charged with toxic hypergolic liquid rocket propellants (hydrazine fuels and nitrogen tetroxide oxidizer), the civilian population near these sites must be protected from accidental atmospheric releases of these toxic propellants in the event of a transportation, handling, or storage accident. In addition, these same propellants are used in support of other operational and planned weapons system (e.g., Minutemen III and M-X missile) and space launch vehicles (e.g., Space Shuttle).

Procedures for predicting toxic vapor corridors for an accidental release of either hydrazine fuel or nitrogen tetroxide oxidizer were developed in the early 1960s by the Air Force Cambridge Research Laboratory. At this time, the type of release anticipated by the Air Force at these sites was a single propellant spill, and the predictions of the toxic vapor corridors upon release into the atmosphere were based on the evaporation of the single propellant and on its subsequent dispersion. The techniques developed by the Air Force Cambridge Research Laboratory to determine these toxic corridors were incorporated into the operational procedures when the Titan II was deployed.

In 1980, a Titan II accident occurred near Damascus, Arkansas in which the scenario was much different than the one for which the toxic hazard corridor calculation procedures were developed. Leaking fuel within the silo eventually made contact with the oxidizer on board a Titan II, leading to a violent explosion which sent combustion products and possibly some unreacted propellant several thousand feet in to the air, where the atmospheric dispersion process began. This effort is designed to characterize the interactions of hypergolic liquid rocket propellants and to provide

information pertinent to the development of a model which would describe the transport and diffusion process of the airborne combustion products and unreacted propellant vapors resulting from a catastrophic accident involving hypergolic liquid rocket propellants.

SECTION II

COMPILATION OF BACKGROUND INFORMATION

Information with respect to hypergolic interactions between hydrazine fuels and nitrogen tetroxide oxidizers was obtained from a variety of sources. The Air Force Project Officer supplied several literature references which were invaluable in determining critical fireball parameters such as fireball size, duration, and thermal energy. Technical reports, documents, and literature sources relative to the identification of combustion products, fireball generation, and chemical reaction kinetics in the reaction between the hypergolic liquid rocket fuels were identified through a NASA-RECON and a Chemical Abstracts computer search.

Past experiments involving reactions between hydrazine fuels and nitrogen tetroxide/nitrogen dioxide oxidizers have been identified in the literature reference articles, including the analysis of the Project Pyro tests. The results of these experiments have identified vapor phase and condensed phase reaction products resulting from the mixing of two hypergols and have generated representative explosive yield characteristics for the hypergolic reaction. In addition to the established combustion products of aerazine-50 with nitrogen tetroxide (which include nitrogen, carbon dioxide, and water vapor), approximately 60 additional chemical species resulting from this hypergolic fuel-oxidizer combustion have been reported in the literature. While the identification and quantification of all such chemical reaction products is too exhaustive and detailed for the present task, some of these chemical species may be important components in the combustion fireball due to thermal or toxicity considerations. Dimethylnitrosamine (NDMA), for example, is an expected and confirmed product from the nitrogen tetroxide - diethyl hydrazine reaction¹ and also is a known carcinogen.

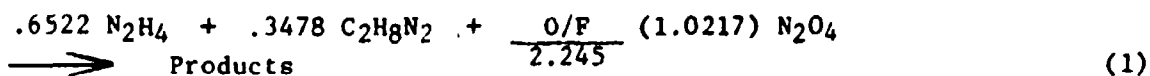
Information from past accidents which involved reactions of hypergolic rocket propellants has also been evaluated with respect to the thermophysical analysis pertinent to the present effort. Results from the Atlas/Centaur Launch Hazards Assessment Program and the Titan II accident in 1980 were included in this evaluation.

SECTION III

THE CHEMISTRY OF THE HYDRAZINE/NITROGEN TETROXIDE BIROPELLANT SYSTEM

The hypergolic combination of hydrazine-type fuels (including hydrazine, monomethylhydrazine [MMH], 1, 1 - dimethylhydrazine [UDMH], and aerazine-50 (A-50, a 50:50 mixture of hydrazine and UDMH by weight) with nitrogen tetroxide [NTO] oxidizers are used in current propulsion systems such as the Titan II Weapons System and the Shuttle Transportation System. This is of the high specific impulse imparted to the launch vehicle by the chemical energy released upon mixing the hypergols in the rocket engine.

The stoichiometric reaction between aerazine-50 and nitrogen tetroxide (the biropellant system used in the Titan II Weapons System) may be represented by the following equation²:



where O/F is the oxidant-fuel mass ratio (2.245 for stoichiometric combustion) and the products of combustion consist primarily of water vapor (H_2O), nitrogen gas (N_2), carbon monoxide (CO), carbon dioxide (CO_2), hydrogen gas (H_2), and hydroxide radical (OH). The available chemical energy from reacting one gram mole of aerazine-50 (.6522 mole hydrazine + .3478 mole UDMH) with 1.02 moles of nitrogen tetroxide at 25°C (298°K) is approximately 1.54×10^5 calories (6.63×10^3 BTU per pound aerazine-50 reacted). This value was calculated from the standard heats of formation of chemical reactants and gaseous reaction products for the stoichiometric hypergolic reaction referenced at 298°K , and will be discussed in more detail in Section IV.

In addition to the formation of the gaseous combustion products described above for a stoichiometric reaction between aerazine-50 fuel and nitrogen tetroxide oxidizer, several competing side reactions occur upon mixing of the two hypergols, and over 50 chemical species have been isolated and identified either as chemical intermediates or condensed phase reaction products in the A-50/NTO hypergolic reaction.

A list of reported secondary chemical reaction products that result from the interaction of Aerazine-50 fuel and nitrogen tetroxide oxidizer is included in Table I. Some of these side products (such as hydrazine nitrate and hydrogen azide) have been identified as the reaction condensates responsible for the "hard start" and "popping" phenomena characteristic of hydrazine-NTO pulsed rocket engines^{3,4,5}. While these particular chemical residues affect engine performance and ignition threshold, the instability of these compounds at elevated temperatures suggests their absence in a hypergolic fireball resulting from a propellant accident during transportation or handling. The hydrazine nitrates and azides; therefore, are not seen to be airborne toxins in an accidental hypergolic explosion. Other chemical reaction products are more stable, especially at lower temperatures (500°K), and the presence of these compounds in a hypergolic fireball may significantly impact the toxic vapor corridors for a bipropellant accident scenario. The chemical species in this category include dimethylnitrosamine (NDMA), methyl amine, dimethyl amine, formaldehyde, hydrogen cyanide, ammonia, and formaldehyde dimethylhydrazine (FDH). In addition to these reaction products, unreacted propellant vapors (hydrazine vapor, UDMH vapor, nitrogen dioxide) resulting from incomplete combustion and volatilization of excess propellant will also pose a health hazard upon atmospheric dispersion, since both the hydrazine fuel and nitrogen tetroxide oxidizer are extremely toxic, in both the liquid and vapor states.

Most of the reaction products cited in the literature and listed in Table I can be accounted for by one or more of the following chemical reaction mechanisms.

TABLE I

REACTION PRODUCTS IDENTIFIED IN THE AEROZINE-50
NITROGEN TETROXIDE REACTION

No.	Compound Name	Molecular Formula	Reference
1	nitrogen	N_2	1,3,6
2	hydrogen	H_2	3,6
3	water	H_2O	3,6
4	oxygen	O_2	3,6
5	carbon dioxide	CO_2	1,3
6	carbon monoxide	CO	1,3
7	ammonia	NH_3	1,3,6
8	nitrogen dioxide	NO_2	1,3
9	nitrous oxide	N_2O	3,6
10	nitric oxide	NO	3,6
11	hydroxide	OH	2
12	monatomic hydrogen	H	2
13	monatomic oxygen	O	2
14	nitrogen trioxide	N_2O_3	2
15	nitric acid	HNO_3	3,6
16	nitrous acid	HNO_2	3,6
17	hydrogen azide	HN_3	3
18	hydrazine azide	$N_2H_5N_3$	3,5
19	methanol	CH_3OH	1,3
20	methyl amine	CH_3NH_2	1
21	dimethyl amine	$(CH_3)_2NH_2$	1

TABLE I (Continued)

REACTION PRODUCTS IDENTIFIED IN THE AEROZINE-50
NITROGEN TETROXIDE REACTION

No.	Compound Name	Molecular Formula	Reference
22	formamide	CNH_2O	1
23	formaldehyde	CH_2O	3
24	nitrosamine	NH_2NO	3,6
25	dimethylnitrosamine	$(\text{CH}_3)_2\text{NNO}$	1,3
26	dimethylformamide	$(\text{CH}_3)_2\text{NCO}$	1
27	methylnitrosamine	HCH_3NNO	1
28	hydrazine nitrate	$\text{N}_2\text{H}_5\text{NO}_3$	1,3,4,7
29	hydrazine dinitrate	$\text{N}_2\text{H}_4\cdot 2\text{HNO}_3$	3,5
30	hydrazine nitrite	$\text{N}_2\text{H}_5\text{NO}_2$	3,5
31	dimethylhydrazine nitrate	$(\text{CH}_3)_2\text{NH}_3\text{NO}_3$	1,3
32	ammonium nitrate	NH_4NO_3	3,6
33	ammonium azide	NH_4N_3	3
34	ammonium nitrite	NH_4NO_2	3
35	formaldehyde dimethylhydrazone	$\text{CH}_2\text{NN}(\text{CH}_3)_2$	3
36	tetramethyl tetrazine	$(\text{CH}_3)_4\text{N}_4$	3
37	tetrazine	H_4N_4	3
38	formaldehyde monomethylhydrazone	$\text{CH}_2\text{NNHCH}_3$	3
39	triazine	H_3N_3	3
40	azine	H_2NNNH	3
41	monomethylhydrazine	CH_3HNNH_2	3
42	methyl azide	CH_3N_3	3

TABLE I (Concluded)

REACTION PRODUCTS IDENTIFIED IN THE AEROZINE-50
NITROGEN TETROXIDE REACTION

No.	Compound Name	Molecular Formula	Reference
43	nitromethane	CH_3NO_2	3
44	methyl ammonium nitrate	$\text{CH}_3\text{NH}_3\text{NO}_3$	3
45	nitrosohydrazine	$\text{N}_2\text{H}_3\text{NO}$	3
46	diazomethane	CH_2N_2	3
47	tetramethylhydrazine	$(\text{CH}_3)_4\text{N}_2$	8
48	methyl nitrite	CH_3NO_2	3
49	methane	CH_4	3
50	ethane	C_2H_6	3
51	propane	C_3H_8	3
52	acetylene	C_2H_2	3
53	hydrogen cyanide	HCN	3
54	formic acid	HCOOH	3
55	cyanic acid	HOCN	3
56	butadiene	C_4H_6	3
57	ethyl azide	$\text{C}_2\text{H}_5\text{N}_3$	3
58	ethylene	C_2H_4	3
59	nitrilohydrazine	CNN_2H_5	3

A. FREE RADICAL REACTION

The oxidant, N_2O_4 , or more precisely the monomer NO_2 is a molecule with an unpaired electron and is thus capable of forming free radicals. The NO_2 free radical can dimerize, add to double bonds, abstract hydrogen, and "activate" other chemical species for further chemical reactions. Figure 1 details a reaction mechanism between hydrazine type fuels and nitrogen tetroxide oxidizer through a NO_2 -free radical intermediate.

For the hydrazine reactant A ($R = H$, $R' = H$), the intermediate products are ammonia (E), nitrosamine (F) and ammonium nitrate (G).

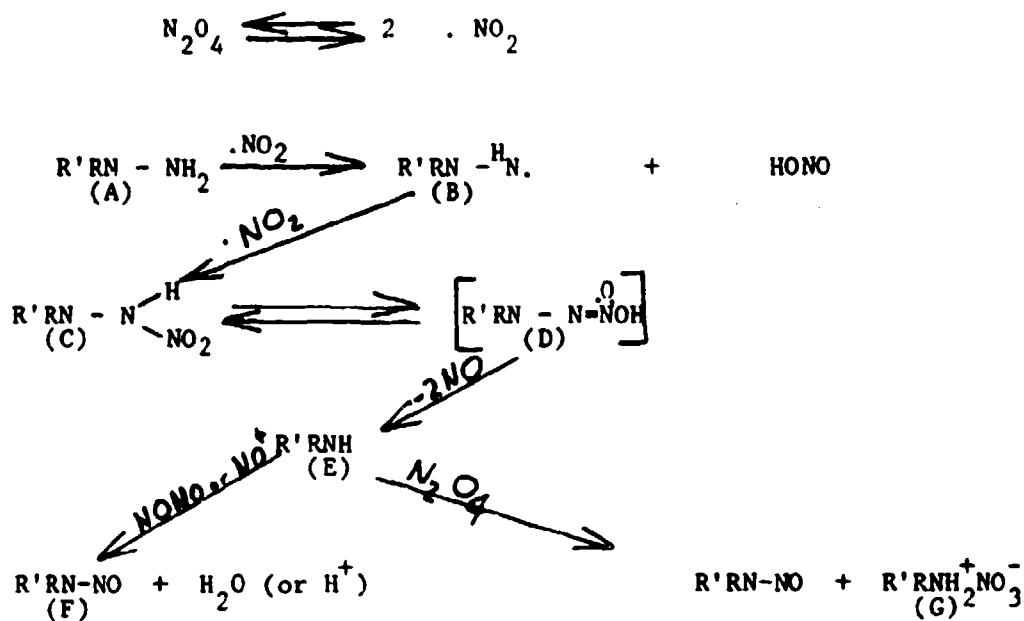
For the monomethyl hydrazine reactant A ($R = H$, $R' = CH_3$) the intermediate products are monomethyl amine (E), methylnitrosamine (F), and methyl ammonium nitrate (G).

For the 1, 1-dimethylhydrazine reactant A ($R = CH_3$, $R' = CH_3$), the intermediate products are dimethyl amine (E), dimethylnitrosamine (F), and dimethyl ammonium nitrate (G).

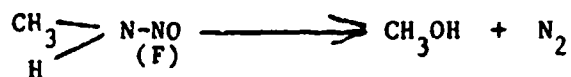
Note that only dimethylnitrosamine is stable upon the oxidation by N_2O_4 . Nitrosamine readily decomposes to water and nitrogen, and monomethylnitrosamine decomposes to methanol and nitrogen.

B. NITROSATION REACTION

Figure 2 shows a postulated mechanism and reaction products resulting from the nitrosation of hydrazines by nitrosonium ion (NO^+), formed from the ionization of nitrogen tetroxide which is promoted by donor solvents such as amines and hydrazines.



if $\text{R}' = \text{CH}_3$ and $\text{R} = \text{H}$, then



if $\text{R} = \text{R}' = \text{H}$, then

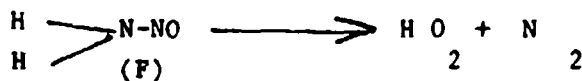


Figure 1. Proposed Free Radical Mechanism for Reaction of N_2O_4 with Hydrazine (Reproduced from Reference 1)

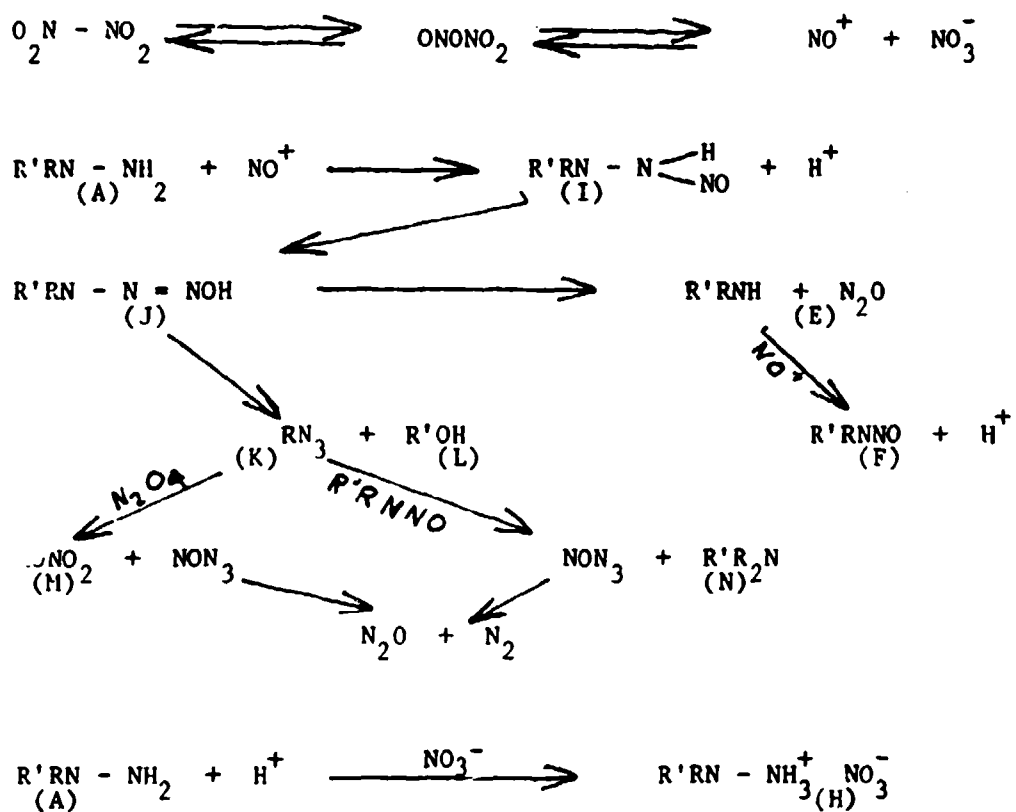
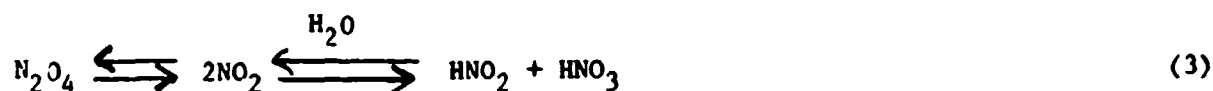
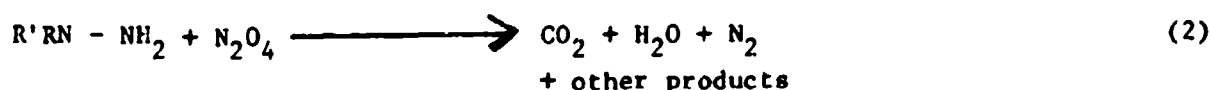


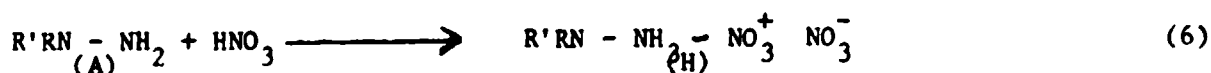
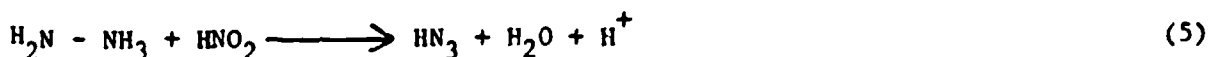
Figure 2. Proposed Nitrosation Mechanism for Reaction of N_2O_4 with Hydrazines (Reproduced from Reference 1)

This reaction also accounts for the formation of substituted amines (products E + N), nitrosamines (product F) and methanol or water (product L). It also indicates the formation of nitrosohydrazine (product I), the azides (methyl and hydrogen, product K) and methyl nitrate or nitric acid (product M). The substituted hydrazinium nitrates (product H) are formed from the reaction of substituted hydrazines with nitric acid.

Several of these species may also form via a simpler mechanism. Since water is a reaction product of the hydrazine/nitrogen tetroxide reaction, the water generated by this hypergolic reaction may react with unreacted nitrogen tetroxide to form nitrous acid and nitric acid, which may subsequently react with the substituted hydrazines to form azides, nitrosamines, and hydrazinium nitrates.



for $\text{R}' = \text{R} - \text{H}$,



The occurrence of the other reaction products in the aeroxine-50/nitrogen tetroxide reaction can be best explained by the oxidation of methanol by NO_2 (or N_2O_4) which produces formaldehyde. The formaldehyde can further react to form acetic acid, formamide or an N-substituted formamide, formic acid, and formaldehyde dimethyl hydrazone¹.

In general, the appearance and relative composition of the reaction products described above depend on the oxidizer/fuel ratio, reaction temperature, reaction pressure, degree of mixing of oxidizer and fuel, and geometric and temporal mixing conditions (such as surface area and wall effects, as well as propellant addition rates). As will be subsequently described, few of these secondary reaction products are predicted by chemical equilibrium considerations; most products identified in a reaction mixture therefore are frozen in a nonequilibrium state due to kinetic barriers. Since activation energies for the various reaction pathways are not readily available, prediction of the absolute amounts of these secondary products in a given hypergolic reaction is difficult at best.

C. ATMOSPHERIC OXIDATION OF HYPERGOLIC ROCKET FUELS

Hypergolic liquid rocket fuel (hydrazine, MMH, UDMH) will react with atmospheric oxygen to produce some of the same oxidation products identified in the fuel/nitrogen tetroxide reactions. Because oxygen is a weaker oxidizer than NTO, the stable oxidation products resulting from the interaction of the hydrazine fuels with air are intermediates in the hydrazine/NTO reaction. For example, formaldehyde dimethyl hydrazone (FDH) has been identified as a minor oxidation product or intermediate in the UDMH/NTO reaction but as the major oxidation product in the UDMH/air reaction. These air oxidation products are important in catastrophic accidents in which unreacted liquid fuel or fuel vapors are exposed to the air, particularly upon atmospheric dispersion of unreacted fuel vapors.

1. Hydrazine Autoxidation

Hydrazine reacts with atmospheric oxygen to produce nitrogen and water according to Equation (7).



A side product of this air oxidation of hydrazine vapor is gaseous ammonia, and the rate of the main reaction, as well as the side reaction producing ammonia has been determined to be strongly dependent on surface area and geometric factors⁹.

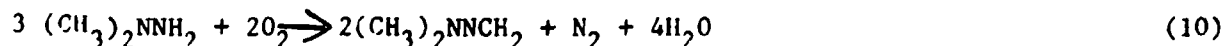
Hydrazine may also decompose in the absence of air to form ammonia, nitrogen, and hydrogen according to several pathways, the most generally accepted on is represented in Equation (9).



This reaction, often termed hydrazine monodecomposition, occurs only in the presence of an appropriate catalyst (e.g., metal surfaces) or upon sparking or detonation of vapor mixtures^{6,10}. Thus, unreacted hydrazine vapors may be expected to form ammonia, nitrogen, and hydrogen gas with the release of thermal energy under conditions in which the accidental mixing of hypergolic rocket fuels favors a detonation reaction or explosion.

2. Oxidation of Substituted Hydrazines

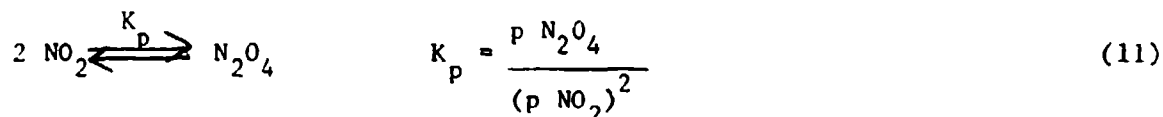
The major oxidation products identified in the MMH/air reaction are formaldehyde monomethyl hydrazone (FMH), methane, methanol, nitrogen, and water¹¹. The reaction between UDMH and air produces FDH, nitrogen, and water according to the stoichiometry in Equation (10).



Diazomethane, dimethylamine, ammonia, and NDMA have been identified as minor products in the UDMH/air reaction¹¹.

D. ATMOSPHERIC REACTIONS OF HYPERGOLIC ROCKET OXIDIZERS

Unreacted liquid rocket oxidizer (NTO) may vaporize during an accident involving hypergolic rocket propellants to product nitrogen tetroxide vapors and nitrogen dioxide vapors. The proportion of nitrogen tetroxide to nitrogen dioxide in the vapor phase is controlled by the equilibrium constant K_p for the reaction:



Where $p \text{ N}_2\text{O}_4$ = partial pressure N_2O_4 vapor at equilibrium
 $p \text{ NO}_2$ = partial pressure NO_2 vapor at equilibrium

The equilibrium constant K_p for the association of two molecules of nitrogen dioxide gas into one molecule of nitrogen tetroxide gas is temperature-dependent and can be calculated by the Gibbs free-energy function for the association reaction [Equation (11)]:

$$\Delta G^\circ = -RT \ln K_p = -13600 + 412.6 T \quad (12)$$

Where R = gas constant (1.987 cal/mole = °K)
 K_p = association equilibrium constant (1/atm)
 T = gas temperature (°K)
 ΔG° = Gibbs free energy (calories/mole)

The equilibrium mole fractions of nitrogen tetroxide gas and nitrogen dioxide gas as a function of temperature as calculated from Equations (11) and (12) are presented in Table II. In this case, the mole fractions of nitrogen

oxide vapors (NO_2 or N_2O_4) are equal to the partial pressures of the vapors at one atmosphere total pressure. The percent of dissociation of nitrogen tetroxide dimer to nitrogen dioxide monomer, as defined in Equation (13), is also presented in Table II. Thus, above 100°C (373°K), unreacted nitrogen tetroxide gas is virtually completely dissociated into nitrogen dioxide gas¹².

$$\text{Percent Dissociation} = \frac{p \text{ NO}_2 \times 100}{p \text{ NO}_2 + 2p \text{ N}_2\text{O}_4} \quad (13)$$

TABLE II. EQUILIBRIUM COMPOSITION OF NITROGEN TETROXIDE AND NITROGEN DIOXIDE IN THE VAPOR PHASE AS A FUNCTION OF ABSOLUTE TEMPERATURE

($P_{\text{Total}} = 1$ Atmosphere)

Temperature $^\circ\text{K}$	Mole Fraction N_2O_4	Mole Fraction NO_2	Percent Dissociation
298	.698	.302	18
313	.539	.461	30
323	.426	.574	40
373	.066	.934	88

Oxidizer vapors evolved during a hypergolic propellant accident, which will include both N_2O_4 and NO_2 gases, will react with the atmospheric components of air during fireball generation and aerial dispersion. These vapors are expected to react with molecular oxygen to produce a mixture of nitrogen oxides (NO_x) which may include nitrogen trioxide (NO_3 ; $x = 3$), dinitrogen trioxide (N_2O_3 ; $x = 3/2$) and dinitrogen pentoxide (N_2O_5 ; $x = 5/2$). They will also react with atmospheric water vapor to produce both nitrous acid (HNO_2) and nitric acid (HNO_3). The latter phenomenon is known as the acid rain effect. Vaporized rocket oxidizer may also react with any hydrocarbon pollutants in the atmosphere, and these interactions are detailed in Reference 13.

SECTION IV

THERMOCHEMICAL ANALYSIS OF A HYPERGOLIC REACTION

Upon mixing of the hypergolic rocket propellant (A-50 and NTO) during an accidental spill or missile tank rupture, the chemical energy of the propellants is converted into thermal energy used to heat the hypergolic combustion products, to vaporize excess unreacted propellant, and to heat the surroundings in the vicinity of the accident. The thermal energy of the resultant fireball, as well as a measure of the time-dependent energy release of the fireball (heat flux) upon fireball generation and lift-off, are important in the quantification of the release height of the chemical components contained in the fireball and the subsequent deposition pattern upon aerial dispersion.

Thermochemical analysis for hypergolic fireballs were calculated for three separate cases: (1) Fireball combustion products were identified and adiabatic flame temperatures were calculated, using theoretical thermodynamic combustion properties of the hypergolic propellants and the gaseous reaction products; (2) Where the oxidizer to fuel ratio was far removed from stoichiometric combustion, the chemical reaction was treated as a nonequilibrium condition, in which the resultant thermal energy of the fireball was used to heat and vaporize the excess propellant; and (3) The time - temperature profile of a hypergolic fireball was calculated, assuming radiative heat transfer to the environment. These analyses, as well as the determination of the fireball size, are detailed in the sections that follow.

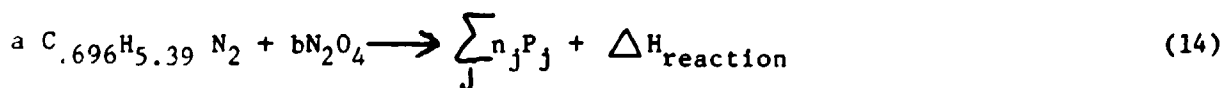
A. ADIABATIC FLAME TEMPERATURE AND CHEMICAL COMPOSITION CALCULATED UNDER EQUILIBRIUM CONDITIONS

Quantification of equilibrium chemical species and calculation of fireball adiabatic temperatures resulting from stoichiometric and nonstoichiometric

reactions of aerazine-50 with nitrogen tetroxide were accomplished using a computer program to calculate complex chemical equilibrium composition (NASA SP-273)¹⁴. The program solves equations by reiteration to minimize the Gibbs free energy of the chemical reaction products and maintain a mass balance between the chemical reactants (hypergolic propellants) and chemical products (combustion products, oxidation products, and unreacted propellants). This particular program has been routinely used at Martin Marietta to calculate rocket performance parameters for Titan launch vehicles employing hypergolic propellants. The program employs approximately 60 possible reaction products resulting from a particular hypergolic propellant combination.

Flame temperatures of hypergolic fireballs were calculated by this program for an adiabatic condition, i.e., conductive, convective, and radiative heat losses to the environment are negligible. In this case, the heat of reaction of combining (a) moles of A-50 with (b) moles of NTO at 25°C (298°K) was used to heat the resultant chemical species in the fireball from 25°C to the final flame temperature T_F .

For the hypergolic chemical reaction:



where:

a = number of moles of A-50 reacted

b = number of moles of NTO reacted

n_j = number of moles of combustion product P_j

$\Delta H_{\text{reaction}}$ = heat evolved from chemical reaction
(calories/mole or BTU/pound)

The adiabatic flame temperature (T_F) is calculated for the hypergolic reaction as follows:

$$\Delta H_{\text{reaction}} = a \Delta H_f^\circ (\text{A-50}) + b \Delta H_f^\circ (\text{NTO}) - \sum_j n_j \Delta H_f^\circ (P_j) \\ = \int_{298}^{T_F} n_j C_{pj} dT \quad (15)$$

For unreacted propellant vapors (P_k) which may be hydrazine vapor, UDMH vapor, NTO vapor or NO_2 vapor depending on the relative amounts of fuel and oxidizer involved in the hypergolic accident (O/F mole ratio is 1.02 for stoichiometric combustion), the enthalpy change from 298°K to T_F includes a phase transition, therefore the final thermochemical equation which includes both gaseous combustion products and vaporized propellant may be written

$$(a + a_1) \Delta H_f^\circ (\text{A-50}) + (b + b_1) \Delta H_f^\circ (\text{NTO}) - \sum_j n_j \Delta H_f^\circ (P_j) \\ = \int_{298}^{T_F} n_j C_{pj} dT + \int_{298}^{T_v} n_k C_{pk} dT + \sum_k n_k \Delta H_{\text{vap}} (P_k) \\ + \int_{T_v}^{T_F} n_k C_{pk} dT \quad (16)$$

Where:

- a_1 = number moles excess A-50 vaporized
- b_1 = number moles excess NTO vaporized
- ΔH_f° = the standard heat of formation of the liquid rocket propellants (A-50 or NTO); or the standard heat of formation of the j^{th} gaseous combustion product
- C_{pj} = the constant pressure heat capacity for the j^{th} gaseous combustion product
- n_k = the number of moles of k^{th} unreacted vaporized propellant

- C_{pk} = the constant pressure heat capacity for the k_{th} unreacted propellant at the temperature interval of interest
 T_v = temperature ($^{\circ}K$) at phase transition
 ΔH_{vap} = latent heat of vaporization at T_v $^{\circ}K$

Computer calculations were performed for oxidizer-to-fuel (O/F) mole ratios between 0.0102 and 510.0. The O/F mole ratio for stoichiometric combustion is 1.02, and the O/F mole ratio for the full inventory of hypergolic propellant contained in the Titan II missile (104,609 pounds aerazine-50 and 207,560 pounds nitrogen tetroxide) is approximately 0.90. The calculations were also performed at several reaction pressures intended to simulate different accident scenarios:

1. Combustion in an Open-Field or Vented Environment

$$P_1 = 1.0 \text{ atm}$$

The hypergolic reaction pressure was defined as 1.0 atmosphere (14.7 psia) for propellant accidents in which the gaseous combustion products were allowed to expand and release in an unconfined space. This analysis would be representative of an open-field propellant spill, or a silo spill in which the blast cover door was removed or vented.

2. Confined Silo Fire with Minimal Explosion Hazard

$$P_2 = 12.56 \text{ atm}$$

This situation is intended to represent a bipropellant accident in a confined Titan II missile silo (700-ton horizontal silo door intact) in which the propellant leak rate is too slow to allow any overpressure conditions in the silo due to deflagration or detonation of the combined hypergolic rocket propellants. In this case, the silo pressure will slowly rise until the 700

ton blast door will be ejected, and the resultant fireball will be subsequently released from the opened silo. The pressure at fireball lift-off time can be calculated from the force required to remove the horizontal silo door as follows:

P_2 = Pressure required to eject silo cover =

$$\frac{\text{Weight Silo Door (Pound)} + 4 \times \text{Shear Force T-Lock Restraint}}{\text{Exposed Surface Area Silo Door}} \quad (17)$$

$$P_2 = \frac{1.4 \times 10^6 \text{ Lb} + 4(5.5 \times 10^5 \text{ Lb})}{954 \text{ Ft}^2} = 2.45 \times 10^4 \text{ Lb/Ft}^2$$

$$P_2 = 185 \text{ psia} = 12.56 \text{ atmospheres}$$

3. Open Silo Hypergolic Explosion

$$P_3 = 1.0 \text{ atmosphere} + P_{\text{over}}$$

This analysis is performed to estimate a large-scale propellant spill in which the propellants spill out of missile tankage and mix in an open silo. In this case the spill and mixing rates of the hypergolic propellants are large enough to initiate a chemical explosion. Detonation reactions between hydrazine-type fuels and nitrogen tetroxide oxidizer have been previously documented in the literature^{15,16}. The analyses for the detonation shock front resulting from the accidental explosion has been calculated, using the geometric conditions present in the Titan II launch tube. The area available for expansion of the shock front in this case is equal to twice the cross-sectional area of the launch tube (expansion in two directions) minus the void cross-sectional area of the missile. This is

$$2(\pi R^2) - 2(\pi R'^2) = 946 \text{ Ft}^2 \quad (18)$$

where:

R = radius of launch tube = 13.2 Feet

R' = radius of missile = 5 Feet

Many different factors can affect the severity of the shock overpressure¹⁵. The most significant of these are:

- a. Total propellant weight
- b. Propellant type
- c. TNT equivalent yield
- d. Geometry of surroundings.

The relevant geometry for an in-silo explosion resulting from the mixing of the two hypergolic propellants has been defined above.

The TNT equivalent yield is a measure of the explosive potential of the detonation reaction, i.e., the TNT yield is the weight fraction of the explosive substance which is equal to the same weight of TNT. In hypergolic explosions between A-50 fuel and NTO oxidizer, a 0.5 percent TNT equivalent yield conservative maximum can be expected from Project Pyro test data¹⁶.

The static peak overpressure for the detonation blast wave is the measured air pressure in the shock front, and is related to the total propellant weight, TNT equivalent yield and reduced distance (λ) by the following equation:

$$\log P_{\text{over}} = -2.349 \log \lambda + 3 \quad (19)$$

where P_{over} = the static peak overpressure (psig) and λ = the reduced distance.

In theory, a given overpressure will occur at a distance from an explosion proportional to the cube root of the energy yield or to the cube root of the explosive weight. Full-scale tests indicate that this relation between distance and energy released holds for explosive yields into the megaton range:¹⁵

$$\lambda = \frac{r}{(\%W)^{1/3}} \quad (20)$$

where r = equivalent silo hemisphere radius

$$\lambda = (946/2\pi)^{1/2} = 12.3 \text{ Feet}$$

and percent W = Equivalent explosive weight involved in hypergolic reaction (does not include unreacted vaporized propellant).

Equation (19), which was valid for 1000-pound Project Priyo test data for reduced distances (λ) between 1.0 and 10.0, can be combined with Equation (20) to give the final static overpressure equation:

$$\log P_{\text{over}} = -2.349 \log \left[\frac{12.3}{(.005 W_b)^{1/3}} \right] + 3 \quad (21)$$

Where W_b = the total liquid propellant weight (pounds) involved in the hypergolic reaction.

From Equation (21), hypergolic reactions involving large quantities of mixed propellants are more catastrophic in nature, resulting in higher static peak overpressures and explosive detonation. As the total propellant weight involved in the hypergolic reaction (W_b) decreases, the peak overpressure decreases and the accident scenario more closely resembles a nonexplosive chemical combustion.

For an accident involving the full inventory of rocket propellant in a properly fueled Titan II missile ($W_b = 3.122 \times 10^5$ Lb) the equivalent yield is 1.56×10^3 Lb TNT, and the calculated peak overpressure is 872 psig (60.3 atmospheres). This pressure was therefore used to calculate the theoretical thermodynamic combustion products and adiabatic flame temperatures resulting from a catastrophic accident involving the full inventory of liquid rocket propellant contained in the Titan II missile (Stage 1 and Stage 2).

4. Confined Silo Hypergolic Explosion

$$P_4 = 12.56 \text{ atmosphere} + P_{\text{over}}$$

The situation in which a catastrophic hypergolic accident occurs in a closed missile silo has been approximated by assuming an initial slow pressure buildup followed by an explosive detonation of mixed propellants. In this case, the maximum silo pressure before ejection of the 700-ton horizontal silo door would be the pressure required to eject the silo cover (12.56 atmospheres) plus the static peak overpressure resulting from the hypergolic explosion. For a catastrophic accident involving the mixing of the full propellant load in a sealed Titan II missile silo, the maximum pressure calculated is $12.56 \text{ atm} + 59.3 \text{ atm overpressure} = 71.9 \text{ atmospheres total pressure}$. This pressure is considered a worst-case explosive condition. In accidents which involve the accidental mixing of hypergolic propellants in a sealed silo, the actual silo pressure will depend on the rate of propellant mixing, and on the configuration of the missile and silo prior to the accident. For example, peak overpressures would be different for conditions in which Stages I and II are confined in the silo than for those conditions which result in the expulsion of Stage I and/or II, plus the reentry vehicle (RV) from the silo. The latter case was typical of the accident scenario near Damascus, Arkansas. The total pressure in the sealed silo prior to fireball lift-off is therefore bounded by the minimum pressure to eject the silo door (12.56 atm) and the maximum pressure due to a hypergolic explosion ($12.56 \text{ atm} + P_{\text{over}}$).

Fifteen computer calculations were performed for various hypergolic combinations simulating an in-silo mixing accident (silo door open or closed) or an open-field accident. A description of the computer input pertinent to these 15 calculations is presented in Table III. Results of these 15 computer runs, referenced by their respective case numbers are found in Appendix A. The first five runs are calculated for an O/F mole ratio of .902 (the ratio used in the fueling and firing of a Titan II missile). These calculations were also performed, assuming thermal interaction of the air present in the silo (125,000 Ft³ air). The total propellant weight was decreased from 3 X 10⁵ pound in Run 1 to 3 X 10² pound in Run 5, while the O/F mole ratio (.90) and weight of silo air (9,475 pound) were held constant.

TABLE III. INPUT TO SP-273 COMPUTER CALCULATIONS
FOR BIPROPELLANT ACCIDENTS

Run No.	Case No.	O/F Mole Ratio	O/F Weight Ratio	Weight A-50 Pounds	Weight NTO Pounds	Weight Air Pounds	P ₁ atm	P ₂ atm	P ₃ atm	P ₄ atm
1	1	.902	2.076	1.046×10^5	2.076×10^5	9.475×10^3	1	12.56	60.3	71.9
2	2	.902	2.890	1.046×10^4	2.076×10^4	9.475×10^3	1	12.56	----	----
3	3	.902	11.04	1.046×10^3	2.076×10^3	9.475×10^3	1	12.56	----	----
4	4	.902	92.57	1.046×10^2	2.076×10^2	9.475×10^3	1	12.56	----	----
5	5	.902	907.8	10.46	20.76	9.475×10^3	1	12.56	----	----
6	6	1.02	2.348	9.247×10^4	2.076×10^5	9.475×10^3	1	12.56	59	70.6
7	19	1.02	2.245	9.247×10^4	2.076×10^5	0	1	12.56	----	----
8	32	0.51	1.122	9.247×10^4	1.038×10^5	0	1	-----	----	----
9	20	0.204	4.49×10^{-1}	9.247×10^4	4.152×10^4	0	1	-----	----	----
10	21	0.102	2.25×10^{-1}	9.247×10^4	2.076×10^4	0	1	-----	----	----
11	23	0.010	2.25×10^{-2}	9.247×10^4	2.076×10^3	0	1	-----	----	----
12	33	2.04	4.49	4.623×10^4	2.076×10^5	0	1	-----	----	----
13	26	5.1	1.123×10^1	1.849×10^4	2.076×10^5	0	1	-----	----	----
14	28	51.0	1.123×10^2	1.849×10^3	2.076×10^5	0	1	-----	----	----
15	30	51.0	1.123×10^3	1.849×10^2	2.076×10^5	0	1	-----	----	----

Results for the full inventory of liquid rocket propellant (3×10^5 pounds) indicate adiabatic flame temperatures of 2916°K, 3180°K, 3340°K, and 3357°K for silo pressures of 1 atmosphere, 12.56 atmospheres, 60.3 atmospheres, and 71.9 atmospheres respectively. The major fireball constituents for this reaction were carbon monoxide, carbon dioxide, hydrogen gas, water vapor, nitric oxide, nitrogen gas, hydroxide radical, and oxygen gas, the proportion of which varied according to the reaction (silo) pressure. As the total propellant weight decreased, the thermal energy of the combustion products was used to heat the silo air. Thus in Case 5, which employed a 1/1000 propellant load (3×10^2 pound), the adiabatic flame temperature was reduced to 323°K at 1 atmosphere pressure and also 323°K at 12.56 atmospheres pressure. The exact quantity of silo air which will interact with the hypergolic rocket fuels will depend on the extent of mixing and fireball lift-off time.

Run number 7 (Case 19) details the computer results for a stoichiometric mixing of hypergolic rocket propellants ($O/F = 1.02$) in the absence of interacting air. The results of this analysis, presented in Figure 3, will be used in thermochemical calculations to be described in subsequent sections. Since no air was allowed to interact with the liquid rocket fuel, the calculated adiabatic flame temperature of 2917°K is independent of the total propellant weight, W_b , as long as the O/F ratio remains constant.

Hypergolic spills which involve an excess of A-50 fuel (Computer Runs 8-11) indicate that the calculated equilibrium chemical species contained in the fireball would be carbon black (C), methane gas (CH_4), hydrogen gas (H_2), and nitrogen gas (N_2).

Spills which involve an excess of NTO oxidizer (Computer Runs 12-15) contain mostly nitrogen gas and oxygen gas as equilibrium fireball components with very small amounts of other chemical species present.

These computer results which involve nonstoichiometric mixing of A-50 fuel and NTO oxidizer are accurate for ideal thermodynamic conditions, i.e., when the Gibbs free energy of the reaction products is minimized. Unfortunately, not all chemical reactions occur naturally and within a reasonable time frame to produce the thermodynamically stable product.

As an allotropic form of carbon, graphite is thermodynamically more stable than a diamond. A diamond, however, does not spontaneously revert to the graphite without extremes of temperature. The difference between the actual chemical composition and the thermodynamically predicted compositions may be attributed to the kinetic barrier or energy of activation for the reaction. Since the nonstoichiometric calculations described above for a mixing of hypergolic fuel and oxidizer do not account for kinetic effects, a more realistic approach to fuel-rich or fuel-lean combustion reactions is presented in the following section.

B. VAPORIZATION OF EXCESS UNREACTED PROPELLANTS CALCULATED UNDER NONEQUILIBRIUM CONDITIONS

Because the NASA SP-273 computer program did not predict propellant vaporization due to kinetic factors, an approach was formulated which allows the vaporization of excess liquid rocket propellant and calculates the final adiabatic flame temperature of the resulting fireball under nonstoichiometric conditions.

In general, the fuel and oxidizer reacted stoichiometrically, according to Equation (1) in Section III, and the thermal energy resulting from this chemical reaction was used to vaporize any excess unreacted propellant. The fireball chemical species for nonstoichiometric conditions, therefore, contained the combustion products calculated for Computer Run 7 (Case 19) and the vaporized excess propellant. Because the chemical thermal energy released from the hypergolic reaction was used to vaporize and heat excess propellant, final adiabatic temperatures were significantly lower than those reported in Section A.

Calculations are provided in this section for the following vaporization conditions:

1. All excess fuel (hydrazine + UDMH) vaporized
2. All excess oxidizer (N_2O_4) vaporized
3. UDMH selective evaporation
4. Hydrazine monodecomposition and UDMH evaporation
5. Oxidizer evaporation and dissociation into NO_2

The exact vaporization condition depends strongly on the nature of the hypergolic accident. Condition 4, for example, would be a more likely result than Condition 1 in cases in which the accident involves an explosion, since the decomposition of hydrazine to ammonia occurs catalytically and rapidly when explosively initiated. Condition 5 is the preferred mechanism for oxidizer

vapor release at temperatures above 373°K (refer to Table II - Section D). UDMH selective evaporation may occur during tank rupture because the vapor pressure of UDMH liquid is significantly higher than hydrazine liquid.

The mathematical development of the thermochemical equation required to predict fireball temperatures and chemical compositions in hypergolic reactions involving an excess of A-50 fuel or NTO oxidizer is presented below:

Define:

- a_1 = # moles hydrazine liquid reacted
- a_2 = # moles UDMH liquid reacted
- a_3 = # moles nitrogen tetroxide liquid reacted
- a_4 = # moles carbon monoxide (CO) formed by combustion
- a_5 = # moles carbon dioxide (CO₂) formed by combustion
- a_6 = # moles hydrogen radical (H) formed by combustion
- a_7 = # moles hydrogen gas (H₂) formed by combustion
- a_8 = # moles water vapor (H₂O) formed by combustion
- a_9 = # moles nitric oxide (NO) formed by combustion
- a_{10} = # moles nitrogen gas (N₂) formed by combustion
- a_{11} = # moles hydroxide radical (OH) formed by combustion
- a_{12} = # moles oxygen gas (O₂) formed by combustion
- a_{13} = # moles hydrazine vaporized
- a_{14} = # moles UDMH vaporized
- $2a_{15}$ = # moles NO₂ formed from a_{15} moles N₂O₄
- a_{16} = # moles NH₃ formed from hydrazine decomposition
- a_{17} = # moles H₂ formed from hydrazine decomposition
- a_{18} = # moles N₂ formed from hydrazine decomposition
- a_{19} = # moles N₂O₄ vaporized
- α = Oxidizer/Fuel mole ratio
- p' = Percent Mixing (Fraction of excess propellant vaporized)
- X = moles of excess fuel (A-50)
- Y = moles of excess oxidizer (NTO)
- f = fraction excess N₂O₄(g) dissociated into 2NO₂(g) at temperature T(°K)

For an adiabatic process,

$$\Delta H_f^{\circ} \text{ reactants} = \Delta H_f^{\circ} \text{ products} + \int_{298}^{T_F} C_p dT \text{ (products)}$$

where T_F = adiabatic flame temperature

C_p° = low pressure heat capacity of products

$$\text{for } C_p^{\circ} = A + BT + CT^2 + DT^3 \quad \left\{ \begin{array}{l} C_p^{\circ} \text{ in cal/mole } ^{\circ}\text{K} \\ T \text{ in } ^{\circ}\text{K} \end{array} \right.$$

then upon integration: $\Delta H_f^{\circ} \text{ reactants} =$

$$\Delta H_f^{\circ} \text{ products} + AT_F + \frac{B}{2} T_F^2 + \frac{C}{3} T_F^3 + \frac{D}{4} T_F^4 + E \quad (22)$$

$$\text{where } E = -A(298) - \frac{B}{2} (298)^2 - \frac{C}{3} (298)^3 - \frac{D}{4} (298)^4$$

The low-pressure heat capacities for fireball reaction products, as well as the standard free energies of formation for reactants and products, were obtained from a variety of sources^{14,17,18} and are presented in Table IV. The vapor-phase heat capacity for UDMH was not readily available in the literature so it was estimated by using Dobratz's Equation¹⁹.

Note that the sensible and latent heats for propellant vaporization are not required in this analysis, since these heats are already included in the heats of formation of the propellant vapors at 298°K (ΔH_f° for species ^a13, ^a14, and ^a19).

TABLE IV. THERMOCHEMICAL PROPERTIES FOR HYPERGOLIC PROPELLANTS
AND REACTION PRODUCTS

Coef- ficient	Species*	ΔH_f°	Temp Range °K	A	B 10^2	C 10^5	D 10^9	E 10^{-3}
a_1	$N_2H_4(1)$	12054	-----	-----	-----	-----	-----	-----
a_2	UDMH(1)	12339	-----	-----	-----	-----	-----	-----
a_3	$N_2O_4(1)$	-4676	-----	-----	-----	-----	-----	-----
a_4	CO	-26416	273-3700	6.480	0.1566	-.0239	0	-1.998
a_5	CO ₂	-94052	273-3700	6.393	1.0100	-.3405	0	-2.324
a_6	H	52094	1000-5000	4.968	0	0	0	-1.480
a_7, a_{17}	H ₂	0	273-3700	6.424	0.1039	-.0078	0	-1.960
a_8	H ₂ O	-57798	273-3700	6.970	0.3464	-.0484	0	-2.227
a_9	NO	21600	273-3700	6.462	0.2358	-.0770	.0873	-2.024
a_{10}, a_{18}	N ₂	0	273-3700	6.529	0.1488	-.0227	0	-2.010
a_{11}	OH	9625	1000-5000	5.785	0.1906	-.0386	.0273	-1.805
a_{12}	O ₂	0	273-3700	6.732	0.1505	-.0179	0	-2.071
a_{13}	N_2H_4	22434	1000-5000	10.12	1.85	-.6680	1.119	-3.780
a_{14}	UDMH	20705	0-2000	4.06	6.54	-2.18	0	-3.921
a_{15}	NO ₂	7960	273-1500	5.481	1.366	-.842	1.88	-2.170
a_{16}	NH ₃	-11040	273-1500	6.586	0.6126	.2366	-1.598	-2.253
a_{19}	N_2O_4	2114	273-1500	7.945	4.46	-2.71	0	-4.109

ΔH_f° = heat of formation (calories/mole)

$$C_p = A + BT + CT^2 + DT^3 \text{ (calories/mole } ^\circ K)$$

*Species are gaseous unless otherwise noted by (1).

For example:

$$\Delta H_f^0 \text{ hydrazine vapor } (298^\circ\text{K}) = \Delta H_f^0 \text{ hydrazine liquid } (298) + \Delta H_{\text{vap}}^{298} \quad (23)$$

$$\text{and } \Delta H_{\text{vap}}^{298} = \Delta H_{\text{vap}}^{\text{NBP}} + C_p^l (T_B - 298) - C_p^v (T_B - 298) \quad (24)$$

therefore

$$\Delta H_f^0 (298, v) = \Delta H_f^0 (298, l) + C_p^l (T_B - 298) + \Delta H_{\text{vap}}^{\text{NBP}} - C_p^v (T_B - 298)$$

where l = liquid phase
 v = vapor phase
 NBP = normal boiling point
 T_B = temperature at boiling

Coefficients for a stoichiometric reaction of A-50 fuel and NTO oxidizer were determined from Equation (1), Section III for the reactants (hydrazine, UDMH, and NTO), and from the computer output for stoichiometric combustion (Figure 3) for the normal combustion products. These coefficients are:

a ₁ = .6522	a ₂ = .3478	a ₃ = 1.0217
a ₄ = .3807	a ₅ = .3149	a ₆ = .1755
a ₇ = .3570	a ₈ = 2.087	a ₉ = .0726
a ₁₀ = 1.985	a ₁₁ = .3267	a ₁₂ = .59

Only the major combustion species were included in this analysis, and oxygen (a₁₂) was used to provide a mass balance for the chemical reaction.

TABLE 19

CHEMICAL FORMULA										WEIGHT FRACTION (SEE NOTE)	INITIALITY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N	2	(XXXX)	H	4	(XXXX)								
FUEL	C	2	00000	H	8	00000	N	2	(XXXX)	50000	12100.000	L	298.15	0.0000
UNFUEL	N	2	00000	O	4	00000				50000	11900.000	L	298.15	0.0000
O/F = 2.2450 PERCENT FUEL = 30.8166 EQUIVALENCE RATIO = 1.0017 DENSITY = 0.0000										1.00000	-4676.000	L	298.15	0.0000

THERMODYNAMIC PROPERTIES

P. ATM	1.000
T. DEG K	2918
H. CAL/G	53.5
S. CAL/(G)(K)	3.0162
M. MOL WT	22.448
(DLV/DLP)T	-1.03828
(DLV/DLP)P	1.8176
CP. CAL/(G)(K)	2.0417
GAMMA (S)	1.1173
CPF. CAL/(G)(K)	.4689
SON VEL. M/SEC	1098.9

MOLE FRACTIONS

CO	.06301
CO2	.05210
H	.02952
H2O	.00001
H2	.05926
H2O	.34523
H2	.01260
H2	.32797
O	.01682
O4	.05366
O2	.03980

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WERE NOT MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CARBON FUEL.

C	CO	CO2	CO3	C14	C18	C24	C28	C32	C36	C40	C44	C48	C52	C56	C60	C64	C68	C72	C76	C80	C84	C88	C92	C96	C100	C104	C108	C112	C116	C120	C124	C128	C132	C136	C140	C144	C148	C152	C156	C160	C164	C168	C172	C176	C180	C184	C188	C192	C196	C200	C204	C208	C212	C216	C220	C224	C228	C232	C236	C240	C244	C248	C252	C256	C260	C264	C268	C272	C276	C280	C284	C288	C292	C296	C300	C304	C308	C312	C316	C320	C324	C328	C332	C336	C340	C344	C348	C352	C356	C360	C364	C368	C372	C376	C380	C384	C388	C392	C396	C400	C404	C408	C412	C416	C420	C424	C428	C432	C436	C440	C444	C448	C452	C456	C460	C464	C468	C472	C476	C480	C484	C488	C492	C496	C500	C504	C508	C512	C516	C520	C524	C528	C532	C536	C540	C544	C548	C552	C556	C560	C564	C568	C572	C576	C580	C584	C588	C592	C596	C600	C604	C608	C612	C616	C620	C624	C628	C632	C636	C640	C644	C648	C652	C656	C660	C664	C668	C672	C676	C680	C684	C688	C692	C696	C700	C704	C708	C712	C716	C720	C724	C728	C732	C736	C740	C744	C748	C752	C756	C760	C764	C768	C772	C776	C780	C784	C788	C792	C796	C800	C804	C808	C812	C816	C820	C824	C828	C832	C836	C840	C844	C848	C852	C856	C860	C864	C868	C872	C876	C880	C884	C888	C892	C896	C900	C904	C908	C912	C916	C920	C924	C928	C932	C936	C940	C944	C948	C952	C956	C960	C964	C968	C972	C976	C980	C984	C988	C992	C996	C1000	C1004	C1008	C1012	C1016	C1020	C1024	C1028	C1032	C1036	C1040	C1044	C1048	C1052	C1056	C1060	C1064	C1068	C1072	C1076	C1080	C1084	C1088	C1092	C1096	C1100	C1104	C1108	C1112	C1116	C1120	C1124	C1128	C1132	C1136	C1140	C1144	C1148	C1152	C1156	C1160	C1164	C1168	C1172	C1176	C1180	C1184	C1188	C1192	C1196	C1200	C1204	C1208	C1212	C1216	C1220	C1224	C1228	C1232	C1236	C1240	C1244	C1248	C1252	C1256	C1260	C1264	C1268	C1272	C1276	C1280	C1284	C1288	C1292	C1296	C1300	C1304	C1308	C1312	C1316	C1320	C1324	C1328	C1332	C1336	C1340	C1344	C1348	C1352	C1356	C1360	C1364	C1368	C1372	C1376	C1380	C1384	C1388	C1392	C1396	C1400	C1404	C1408	C1412	C1416	C1420	C1424	C1428	C1432	C1436	C1440	C1444	C1448	C1452	C1456	C1460	C1464	C1468	C1472	C1476	C1480	C1484	C1488	C1492	C1496	C1500	C1504	C1508	C1512	C1516	C1520	C1524	C1528	C1532	C1536	C1540	C1544	C1548	C1552	C1556	C1560	C1564	C1568	C1572	C1576	C1580	C1584	C1588	C1592	C1596	C1600	C1604	C1608	C1612	C1616	C1620	C1624	C1628	C1632	C1636	C1640	C1644	C1648	C1652	C1656	C1660	C1664	C1668	C1672	C1676	C1680	C1684	C1688	C1692	C1696	C1700	C1704	C1708	C1712	C1716	C1720	C1724	C1728	C1732	C1736	C1740	C1744	C1748	C1752	C1756	C1760	C1764	C1768	C1772	C1776	C1780	C1784	C1788	C1792	C1796	C1800	C1804	C1808	C1812	C1816	C1820	C1824	C1828	C1832	C1836	C1840	C1844	C1848	C1852	C1856	C1860	C1864	C1868	C1872	C1876	C1880	C1884	C1888	C1892	C1896	C1900	C1904	C1908	C1912	C1916	C1920	C1924	C1928	C1932	C1936	C1940	C1944	C1948	C1952	C1956	C1960	C1964	C1968	C1972	C1976	C1980	C1984	C1988	C1992	C1996	C2000	C2004	C2008	C2012	C2016	C2020	C2024	C2028	C2032	C2036	C2040	C2044	C2048	C2052	C2056	C2060	C2064	C2068	C2072	C2076	C2080	C2084	C2088	C2092	C2096	C2100	C2104	C2108	C2112	C2116	C2120	C2124	C2128	C2132	C2136	C2140	C2144	C2148	C2152	C2156	C2160	C2164	C2168	C2172	C2176	C2180	C2184	C2188	C2192	C2196	C2200	C2204	C2208	C2212	C2216	C2220	C2224	C2228	C2232	C2236	C2240	C2244	C2248	C2252	C2256	C2260	C2264	C2268	C2272	C2276	C2280	C2284	C2288	C2292	C2296	C2300	C2304	C2308	C2312	C2316	C2320	C2324	C2328	C2332	C2336	C2340	C2344	C2348	C2352	C2356	C2360	C2364	C2368	C2372	C2376	C2380	C2384	C2388	C2392	C2396	C2400	C2404	C2408	C2412	C2416	C2420	C2424	C2428	C2432	C2436	C2440	C2444	C2448	C2452	C2456	C2460	C2464	C2468	C2472	C2476	C2480	C2484	C2488	C2492	C2496	C2500	C2504	C2508	C2512	C2516	C2520	C2524	C2528	C2532	C2536	C2540	C2544	C2548	C2552	C2556	C2560	C2564	C2568	C2572	C2576	C2580	C2584	C2588	C2592	C2596	C2600	C2604	C2608	C2612	C2616	C2620	C2624	C2628	C2632	C2636	C2640	C2644	C2648	C2652	C2656	C2660	C2664	C2668	C2672	C2676	C2680	C2684	C2688	C2692	C2696	C2700	C2704	C2708	C2712	C2716	C2720	C2724	C2728	C2732	C2736	C2740	C2744	C2748	C2752	C2756	C2760	C2764	C2768	C2772	C2776	C2780	C2784	C2788	C2792	C2796	C2800	C2804	C2808	C2812	C2816	C2820	C2824	C2828	C2832	C2836	C2840	C2844	C2848	C2852	C2856	C2860	C2864	C2868	C2872	C2876	C2880	C2884	C2888	C2892	C2896	C2900	C2904	C2908	C2912	C2916	C2920	C2924	C2928	C2932	C2936	C2940	C2944	C2948	C2952	C2956	C2960	C2964	C2968	C2972	C2976	C2980	C2984	C2988	C2992	C2996	C3000	C3004	C3008	C3012	C3016	C3020	C3024	C3028	C3032	C3036	C3040	C3044	C3048	C3052	C3056	C3060	C3064	C3068	C3072	C3076	C3080	C3084	C3088	C3092	C3096	C3100	C3104	C3108	C3112	C3116	C3120	C3124	C3128	C3132	C3136	C3140	C3144	C3148	C3152	C3156	C3160	C3164	C3168	C3172	C3176	C3180	C3184	C3188	C3192	C3196	C3200	C3204	C3208	C3212	C3216	C3220	C3224	C3228	C3232	C3236	C3240	C3244	C3248	C3252	C3256	C3260	C3264	C3268	C3272	C3276	C3280	C3284	C3288	C3292	C3296	C3300	C3304	C3308	C3312	C3316	C3320	C3324	C3328	C3332	C3336	C3340	C3344	C3348	C3352	C3356	C3360	C3364	C3368	C3372	C3376	C3380	C3384	C3388	C3392	C3396	C3400	C3404	C3408	C3412	C3416	C3420	C3424	C3428	C3432	C3436	C3440	C3444	C3448	C3452	C3456	C3460	C3464	C3468	C3472	C3476	C3480	C3484	C3488	C3492	C3496	C3500	C3504	C3508	C3512	C3516	C3520	C3524	C3528	C3532	C3536	C3540	C3544	C3548	C3552	C3556	C3560	C3564	C3568	C3572	C3576	C3580	C3584	C3588	C3592	C3596	C3600	C3604	C3608	C3612	C3616	C3620	C3624	C3628	C3632	C3636	C3640	C3644	C3648	C3652	C3656	C3660	C3664	C3668	C3672	C3676	C3680	C3684	C3688	C3692	C3696	C3700	C3704	C3708	C3712	C3716	C3720	C3724	C3728	C3732	C3736	C3740	C3744	C3748	C3752	C3756	C3760	C3764	C3768	C3772	C3776	C3780	C3784	C3788	C3792	C3796	C3800	C3804	C3808	C3812	C3816	C3820	C3824	C3828	C3832	C3836	C3840	C3844	C3848	C3852	C3856	C3860	C3864	C3868	C3872	C3876	C3880	C3884	C3888	C3892	C3896	C3900	C3904	C3908	C3912	C3916	C3920	C3924	C3928	C3932	C3936	C3940	C3944	C3948	C3952	C3956	C3960	C3964	C3968	C3972	C3976	C3980	C3984	C3988	C3992	C3996	C4000	C4004	C4008	C4012	C4016	C4020	C4024	C4028	C4032	C4036	C4040	C4044	C4048	C4052	C4056	C4060	C4064	C4068	C4072	C4076	C4080	C4084	C4088	C4092	C4096	C4100	C4104	C4108	C4112	C4116	C4120	C4124	C4128	C4132	C4136	C4140	C4144	C4148	C4152	C4156	C4160	C4164	C4168	C4172	C4176	C4180	C4184	C4188	C4192	C4196	C4200	C4204	C4208	C4212	C4216	C4220	C4224	C4228	C4232	C4236	C4240	C4244	C4248	C4252	C4256	C4260	C4264	C4268	C4272	C4276	C4280	C4284	C4288	C4292	C4296	C4300	C4304	C4308	C4312	C4316	C4320	C4324	C4328	C4332	C4336	C4340	C4344	C4348	C4352	C4356	C4360	C4364	C4368	C4372	C4376	C4380	C4384	C4388	C4392	C4396	C4400	C4404	C4408	C4412	C4416	C4420	C4424	C4428	C4432	C4436	C4440	C4444	C4448	C4452	C4456	C4460	C4464	C4468	C4472	C4476	C4480	C4484	C4488	C4492	C4496	C4500	C4504	C4508	C4512	C4516	C4520	C4524	C4528	C4532	C4536	C4540	C4544	C4548	C4552	C4556	C4560	C4564	C4568	C4572	C4576	C4580	C4584	C4588	C4592	C4596	C4600	C4604	C4608	C4612	C4616	C4620	C4624	C4628	C4632	C4636	C4640	C4644	C4648	C4652	C4656	C4660	C4664	C4668	C4672	C4676	C4680	C4684	C4688	C4692	C4696	C4700	C4704	C4708	C4712	C4716	C4720	C4724	C4728	C4732	C4736	C4740	C4744	C4748	C4752	C4756	C4760	C4764	C4768	C4772	C4776	C4780	C4784	C4788	C4792	C4796	C4800	C4804	C4808	C4812	C4816	C4820	C4824	C4828	C4832	C4836	C4840	C4844	C4848	C4852	C4856	C4860	C4864	C4868	C4872	C4876	C4880	C4884	C4888	C4892	C4896	C4900	C4904	C4908	C4912	C4916	C4920	C4924	C4928	C4932	C4936	C4940	C4944	C4948	C4952	C4956	C4960	C4964	C4968	C4972	C4976	C4980	C4984	C4988	C4992	C4996	C5000	C5004	C5008	C5012	C5016	C5020	C5024	C5028	C5032	C5036	C5040	C5044	C5048	C5052	C5056	C5060	C5064	C5068	C5072	C5076	C5080	C5084	C5088	C5092	C5096	C5100	C5104	C5108	C5112	C5116	C5120	C5124	C5128	C5132	C5136	C5140	C5144	C5148	C5152	C5156	C5160	C5164	C5168	C5172	C5176	C5180	C5184	C5188	C5192	C5196	C5200	C5204	C5208	C5212	C5216	C5220	C5224	C5228	C5232	C5236	C5240	C5244	C5248	C5252	C5256	C5260	C5264	C5268	C5272	C5276	C5280	C5284	C5288	C5292	C5296	C5300	C5304	C5308	C5312	C5316	C5320	C5324	C5328	C5332	C5336	C5340	C5344	C5348	C5352	C5356	C5360	C5364	C5368	C5372	C5376	C5380	C5384	C5388	C5392	C5396	C5400	C5404	C5408	C5412	C5416	C5420	C5424	C5428	C5432	C5436	C5440	C5444	C5448	C5452	C5456	C5460	C5464	C5468	C5472	C5476	C5480	C5484	C5488	C5492	C5496	C5500	C5504	C5508	C5512	C5516	C5520	C5524	C5528	C5532	C5536	C5540	C5544	C5548	C5552	C5556	C5560	C5564	C5568	C5572	C5576	C5580	C5584	C5588	C5592	C5596	C5600	C5604	C5608	C5612	C5616	C5620	C56
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The coefficients for unreacted vaporized propellants were determined from the O/F mole ratio (α) and vaporization conditions as follows:

1. Excess Fuel Reactions

$$\text{Define } \alpha = \frac{1.0217}{1 + X}$$

$$X = \frac{1.0217 - \alpha}{\alpha}$$

Case 1. All excess hydrazine and UDMH vaporized

$$\begin{aligned} a_{13} &= \text{moles hydrazine vaporized} = \\ &\beta(.6522X) = \beta(.6664 - .6522\alpha)/\alpha \end{aligned}$$

$$\begin{aligned} a_{14} &= \text{moles UDMH vaporized} = \\ &\beta(.3478X) = \beta(.3553 - .3478\alpha)/\alpha \end{aligned}$$

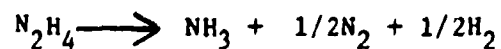
$$a_{15}, a_{16}, a_{17}, a_{18}, a_{19} = 0$$

Case 2. UDMH selective vaporization

$$a_{14} = \beta(.3553 - .3478\alpha)/\alpha$$

$$a_{13}, a_{15}, a_{16}, a_{17}, a_{18}, a_{19} = 0$$

Case 3. Hydrazine decomposition and UDMH vaporization



$$a_{14} = \beta(.3553 - .3478\alpha)/\alpha$$

$$a_{16} = \beta(.6664 - .6522\alpha)/\alpha$$

$$a_{17} = \beta(.3332 - .3261\alpha)/\alpha$$

$$a_{18} = \beta(.3332 - .3261\alpha)/\alpha$$

$$a_{13}, a_{15}, a_{19} = 0$$

2. Excess Oxidant Reactions

$$\text{Define } \alpha = \frac{1.0217 + y}{1}$$

$$y = \alpha - 1.0217$$

$$y = \beta (\alpha - 1.0217)$$

$$a_{15} = \# \text{ moles excess } N_2H_4 = \beta (\alpha - 1.0217)$$

$$2a_{15} = \# \text{ moles vaporized } NO_2 = 2\beta f (\alpha - 1.0217)$$

$$a_{19} = \# \text{ moles vaporized } N_2O_4 = (1-f)\beta (\alpha - 1.0217)$$

$$a_{13}, a_{14}, a_{16}, a_{17}, a_{18} = 0$$

Upon multiplication by known coefficients, integration of the heat capacity function, and collection of terms, the final thermochemical equation for nonstoichiometric hypergolic propellant reactions is:

$$\begin{aligned} & 7375.6 + (a_{13} + a_{16})(12054) + a_{14}(12339) + (a_{15} + a_{19})(-4676) \\ & = -.1595 \times 10^5 + 41.49T + 8.007 \times 10^{-3}T^2 - 1.063 \times 10^{-6}T^3 + 3.807 \times 10^{-12}T^4 \\ & + a_{13}(.186 \times 10^5 + 10.12T + 9.25 \times 10^{-3}T^2 - 2.227 \times 10^{-6}T^3 + 279.8 \times 10^{-12}T^4) \\ & + a_{14}(.186 \times 10^5 + 4.06T + 32.7 \times 10^{-3}T^2 - 7.267 \times 10^{-6}T^3 + 0.0T^4) \\ & + 2a_{15}(.058 \times 10^5 + 5.48T + 6.83 \times 10^{-3}T^2 - 2.807 \times 10^{-6}T^3 + 470 \times 10^{-12}T^4) \\ & + a_{16}(-.133 \times 10^5 + 6.59T + 3.06 \times 10^{-3}T^2 + .788 \times 10^{-6}T^3 + -399.5 \times 10^{-12}T^4) \\ & + a_{17}(-.020 \times 10^5 + 6.42T + .52 \times 10^{-3}T^2 - .026 \times 10^{-6}T^3 + 0.0T^4) \\ & + a_{18}(-.020 \times 10^5 + 6.53T + .74 \times 10^{-3}T^2 - .076 \times 10^{-6}T^3 + 0.0T^4) \\ & + a_{19}(-.020 \times 10^5 + 7.95T + 22.3 \times 10^{-3}T^2 - 9.03 \times 10^{-6}T^3 + 0.0T^4) \end{aligned}$$

(26)

Adiabatic Flame Temperatures and Fireball Compositions were calculated for various O/F ratios, vaporization conditions, and mixing conditions and are presented in Appendix B. Note that when a_{13} , a_{14} , a_{15} , a_{16} , a_{17} , a_{18} , and a_{19} are zero, Equation (26) reduces to a stoichiometric combustion, and yields an adiabatic flame temperature of 2979°K . This temperature is approximately 2 percent higher than that predicted by the NASA SP-273 program because not all the combustion products were considered in this analysis and because the heat capacity data used in this analysis were different than the data used in the computer program.

For a fourfold excess of A-50 fuel (O/F = .204, Analysis 5) the adiabatic flame temperature drops to 1046°K , and the mole fractions of hydrazine vapor and UDMH vapor contained in the fireball are 0.25 and 0.14, respectively. The balance of the chemical constituents in the fireball include primarily water vapor (mole fraction .20) nitrogen gas (mole fraction .19), and oxygen (mole fraction .06); with trace amounts of the remaining combustion products. When calculated for hydrazine decomposition with the same fourfold excess of fuel (O/F = .204, Analysis 6), the calculated fireball temperature is 1523°K (increase in temperature due to thermal stability of ammonia vapor over hydrazine vapor) and the major fireball species are hydrogen gas, water vapor, nitrogen gas, UDMH vapor, and ammonia gas.

For a fourfold excess of NTO oxidizer (O/F = 5.1, Analysis 15), the final calculated adiabatic fireball temperature is 810°K and the fireball composition consists primarily of NO_2 gas (mole fraction .57), nitrogen gas (mole fraction .14) and water vapor (mole fraction .14).

The fireball temperature for the oxidizer-rich reaction is much lower than for the fuel-rich reaction, because energy is required to vaporize excess N_2O_4 liquid ($\Delta H_{\text{vap}} \text{N}_2\text{O}_4 = 6790 \text{ cal/mole NTO}$) and to dissociate the vaporized N_2O_4 molecules into two molecules of nitrogen dioxide gas ($\Delta H_{\text{diss}} \text{N}_2\text{O}_4 = 13,600 \text{ cal/mole NTO}$). As described previously, both of these heats are accounted for in the standard heat of formation of NO_2 gas at 298°K (coefficient a_{15} in Table IV).

Note that excess propellant vaporization is not predicted for oxidizer/fuel ratios larger than 17.7 or smaller than .06 in cases in which both propellant species are 100 percent mixed. In these cases, the heat of reaction is sufficient to raise the excess propellant liquid temperature (sensible heat) but not sufficient to vaporize the excess propellant (heat of vaporization).

C. CALCULATION OF FIREBALL SIZE AND QUANTIFICATION OF HEAT FLUX

The fireball size and heat flux calculations presented here are based on the mathematical description presented by Sandia Laboratories.⁷ This free-field model uses black-body radiation heat losses and continuous expansion of the fireball volume. The convective heat losses and mixing of the reactants and products with the environment are considered negligible during the formation and initial lift-off of the fireball.

1. Theory

The calculations for the fireball formation, using this Sandia Laboratories model, represent the reaction time, t_b , based on a spherical fireball and a hydrodynamic flow model as

$$t_b = 0.6 W_b^{1/6} \quad (27)$$

The reaction time is the time necessary for the mass of hypergolic propellant, W_b , to mix and react to completion. The reaction time, t_b , is also equivalent to the fireball lift-off time. The radius of the fireball, r_b , was determined from the spherical gas volume and the average gas density, $\rho = P(MW)/R'T$,

as

$$r_b = (3/4 \pi \rho)^{1/3} W_b^{1/3} \quad (28)$$

The fireball growth ratio was based on the assumption that the propellant was consumed at a constant rate, R , where

$$R = W/t = W_b/t_b = W_b / (0.6 W_b^{1/6}) = 5W_b^{5/6}/3. \quad (29)$$

The radius of the fireball as a function of time, t , was determined, using Equation (29) to specify the propellant weight and the methodology used to develop Equation (28). This leads to

$$r = (3 R t / 4 \pi \rho)^{1/3} = C t^{1/3} \quad (30)$$

during the time when the propellants are reacting and

$$r = (3 W_b / 4 \pi \rho)^{1/3} t^{1/3}$$

after the reaction has terminated and the fireball has lifted off.

The fireball temperature and rate of energy release were determined from an energy balance that equated the enthalpy of the input propellant minus the energy radiated to the environment to the rate of change of internal energy in the fireball. This can be written as

$$R h_i - \epsilon \sigma A T^4 = d (Wh)_{fb} / dt \quad (31)$$

for the period of time when propellant is being consumed by the reaction and

$$d (Wh)_{fb} / dt = - \epsilon \sigma A T^4 \quad (32)$$

after the reaction is complete.

Equation (31) can be rearranged and simplified using the assumptions and definitions outlined above to give the following nonlinear differential equation that was solved numerically for the temperature during the reaction time ($t' \leq 1$):

$$\frac{dT}{dt'} = \frac{h_1 - h_{fb} - \frac{4 \pi \epsilon \sigma}{1.667 W_b} \left[\frac{3 t' R'}{4 \pi P (MW)} \right]^{2/3} T^{14/3}}{t' C_p} \quad (33)$$

h_1 = H_o reactants, enthalpy of reactants

h_{fb} = $\left[H_o + \int C_p dT \right]$ products, enthalpy of products

ϵ = 1 (black body radiation)

σ = Boltzmann's constant

W_b = weight of propellant

t' = t/t_b = nondimensional time

R' = international gas constant

P = 1 atmosphere, pressure of ambient fireball

(MW) = molecular weight of gaseous products

C_p = $A + B T + C T^2 + D T^3$, specific heat of products

T = absolute temperature

Equation (32) can also be rearranged to solved for the temperature of the fireball after the reduction is completed and the fireball lifts off ($t' \geq 1$).

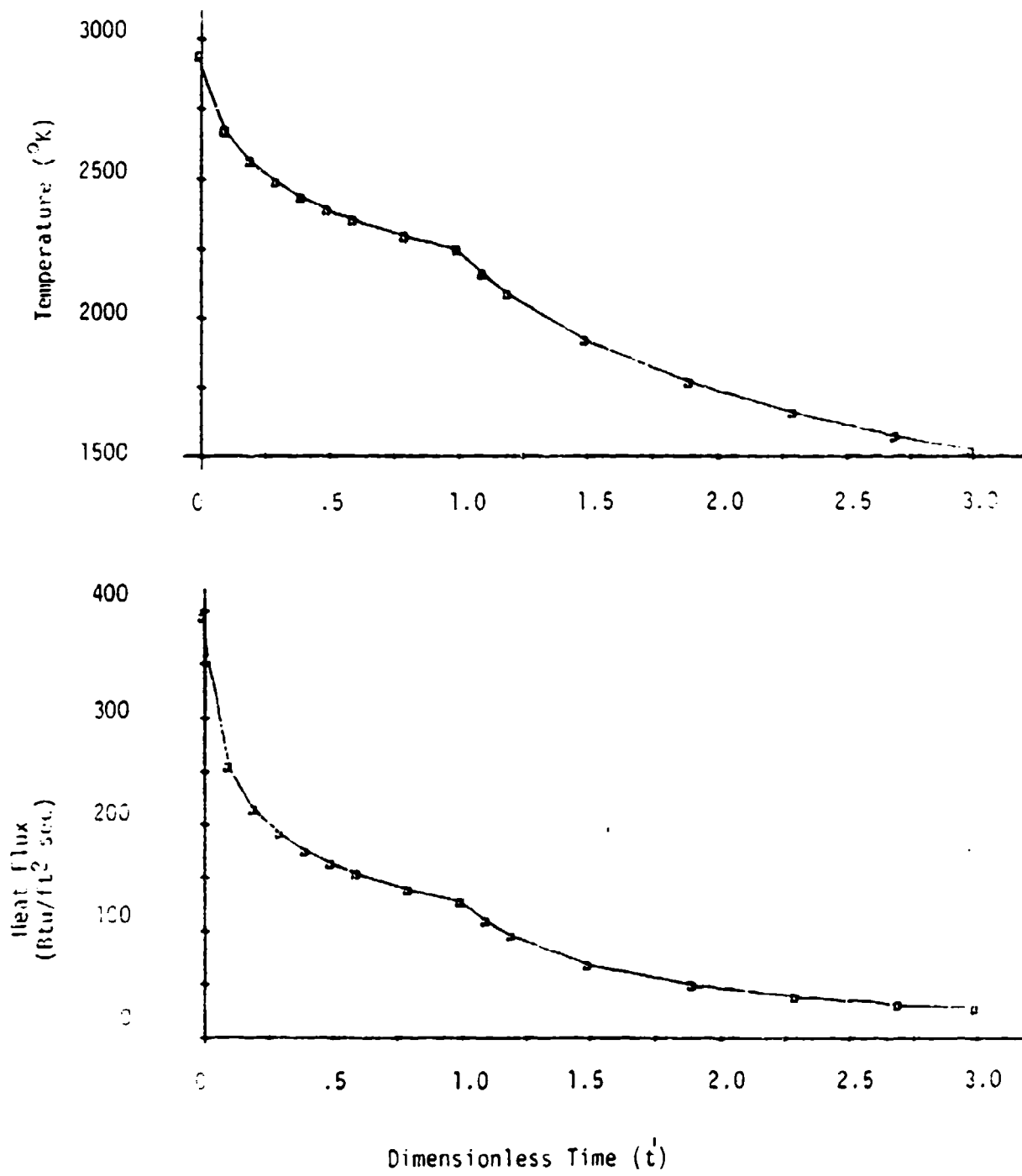
$$\frac{dT}{dt'} = - \frac{4 \pi \epsilon \sigma}{1.66 W_b^{1/6} C_p} \left[\frac{3 R'}{4 \pi P (MW)} \right]^{2/3} T^{14/3} \quad (34)$$

2. Results

Equations (33) and (34) were integrated numerically, using a Fourth Order Runge - Kutta Method. The initial temperature, $T(t') = T(0)$, for the case during the propellant reaction, Equation (33), is the adiabatic flame temperature. The initial condition for Equation (34) which describes the fireball temperature after lift-off, $t' > 1$, was considered to be the solution of Equation (32) at $t' = 1$.

Figure 4 shows the temperature, dimensionless time relationship for 3×10^5 pounds of stoichiometric mixture of N_2O_4 and A-50. The initial temperature of the fireball was calculated to be $2979^\circ K$ and decreased to $2243^\circ K$ at $t' = 1$ which is 4.9 seconds after ignition. The temperature of the rising fireball was calculated to decrease to $1518^\circ K$ at $t' = 3$ or $t = 14.7$ seconds after ignition.

Figure 5 shows the radiant heat flux from the fireball as function of t' for this stoichiometric mixture. The initial value is 393 Btu/Sec ft^2 and decreased to 126 Btu/sec ft^2 at $t' = 1$ after the lift-off, $t' > 1$, the heat flux continues to drop off to approximately 27 Btu/sec ft^2 at $t' = 3$.



Figures 4 and 5. Radiative Fireball Temperature and Heat Loss

$$W_b = 3.00 \times 10^5 \text{ Pounds}$$

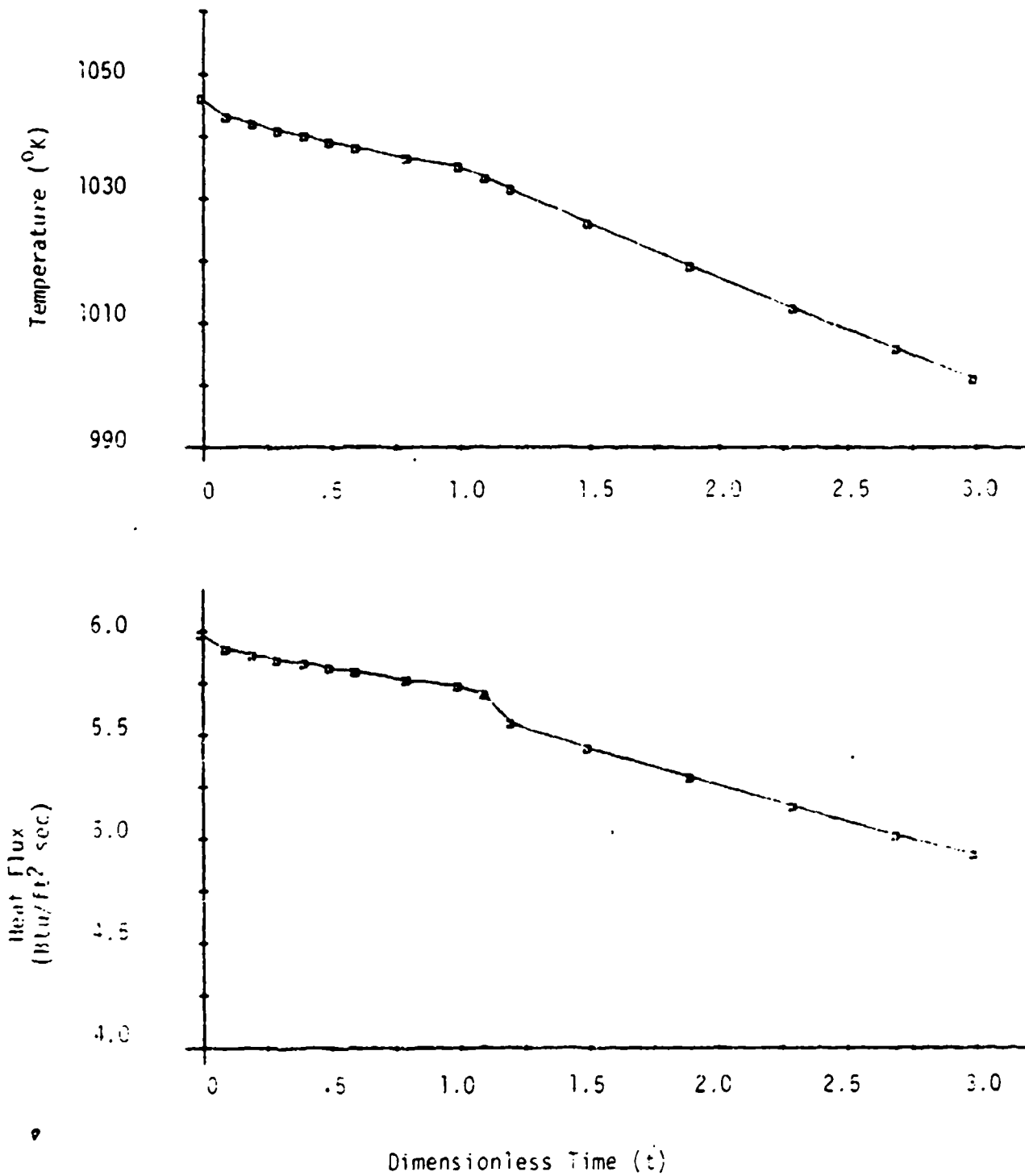
$$O/F = 1.02$$

The temperature and heat flux from a fireball that results from 1.34×10^5 pound mixture of A-50 and N_2O_4 containing a 4X excess of A-50 are shown in Figures 6 and 7, respectively. The initial temperature was $1046^\circ K$ and decreased to $1035^\circ K$ at lift-off, $t' = 1$, which, for this case, occurs 4.3 seconds after ignition. The temperature continues to decrease after lift-off and is $1000^\circ K$ at $t' = 3$ or 12.9 seconds after ignition. The initial heat flux for this case is 6 Btu/sec ft^2 and decreases to 5.7 Btu/sec ft^2 at $t' = 1$. At $t' = 3$, the heat flux has decreased to 4.9 Btu/sec ft^2 . The increased energy needed to evaporate and heat the excess A-50 reduces the energy available to raise the temperature of the fireball and radiate to the environment.

Figures 8 and 9 show the relationships of the temperature and radiant heat flux vs. time for a 2.3×10^5 pound mixture of A-50 and N_2O_4 containing a 4X excess of N_2O_4 . The initial temperature of this system is $810^\circ K$ and decreases to $804^\circ K$ at lift-off, $t' = 1$ or $t = 4.7$ seconds after ignition. The temperature decreases to $786^\circ K$ at $t' = 3$ or 14.1 seconds after ignition. Again, the temperature and heat flux are decreased because of the energy needed to raise the temperature and vaporize the excess N_2O_4 .

3. Conclusion

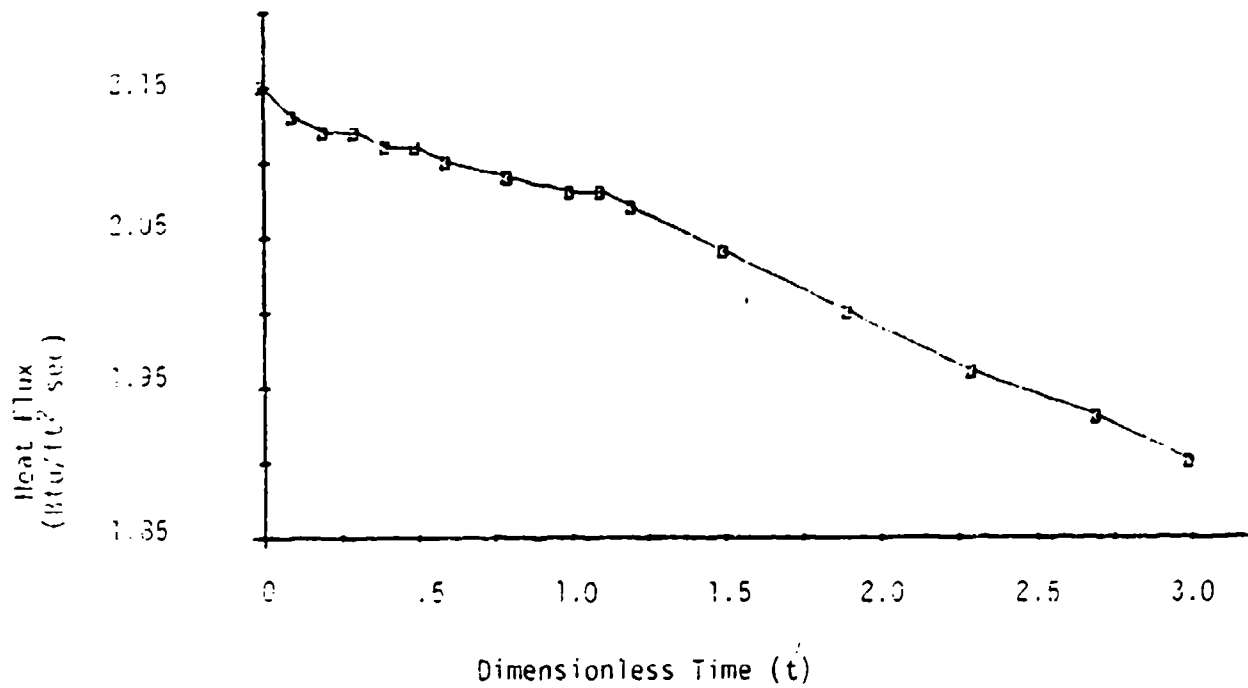
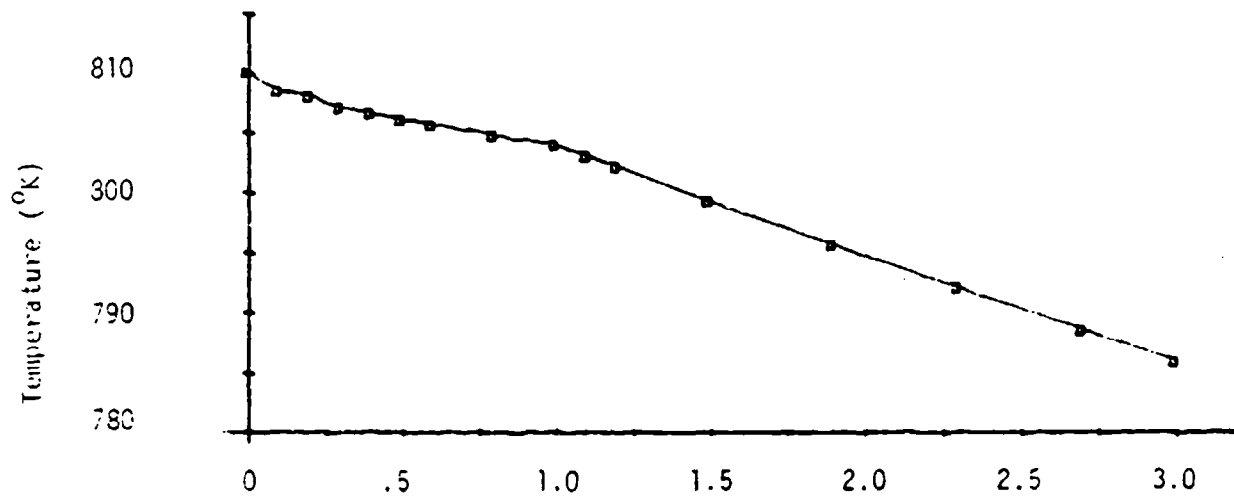
The equations developed and evaluated in this section of the report are general and can be used to determine the temperature and heat flux from a homogeneous fireball when the thermodynamic properties of the reactants and products are known. The maximum temperature and heat flux result from a stoichiometric mixing of the propellants. Excess N_2O_4 reduce both of these properties of the fireball more than excess fuel because of its greater heat of vaporization and specific heat. This causes more energy to be consumed by the components of the reaction mixture; therefore, less energy is released to the environment.



Figures 6 and 7. Radiative Fireball Temperature and Heat Loss

$$W_b = 1.34 \times 10^5 \text{ Pounds}$$

$$O/F = 0.204$$



Figures 8 and 9. Radiative Fireball Temperature and Heat Loss

$$W_b = 2.26 \times 10^5 \text{ Pounds}$$

$$O/F = 5.1$$

SECTION V

REACTIONS OF HYPERGOLIC PROPELLANTS WITH OTHER CHEMICALS

To characterize the explosive hazards of reacting a hypergolic fuel (A-50 or NTO) with other chemicals that may be encountered in a highway or railway accident, the NASA SP-273 computer program was used to predict the theoretical flame temperatures and combustion products resulting from such an accident. Calculations were performed, assuming an equal weight of hypergolic fuel and nonpropellant chemical (O/F weight ratio of 1.0), and were performed at 1.0 atmosphere total pressure which would be indicative of an open-field accident. Because these calculations only consider ideal chemical thermodynamic conditions (and not kinetic parameters as discussed in Section A), the computer output for these reactions contains only the combustion products which would be present at chemical equilibrium.

The chemical reactants used as computer input for these calculations are included in Table V. Computer output for the reactions of hypergolic rocket propellants with these other chemicals are included in Appendix C.

TABLE V. COMPUTER INPUT FOR REACTIONS OF HYPERGOLIC ROCKET
PROPELLANTS WITH OTHER CHEMICALS

Case No.	Fuel*	Oxidant*
34	Methylene Chloride	NTO
35	Ethylene Glycol	NTO
36	Dichloroethane	NTO
37	Liquid Propane	NTO
38	n-Octane	NTO
39	Acetone	NTO
40	Acetylene	NTO
41	Ammonia	NTO
42	A-50	Liquid Oxygen (LOX)
43	A-50	Air (g)
44	A-50	Chlorine
45	A-50	Nitric Acid
46	A-50	Hydrogen Peroxide

* All reactants are in the liquid state unless otherwise noted.

SECTION VI CONCLUSIONS

The purpose of this document is to provide engineering data which will be used to predict the aerial dispersion patterns of chemical reaction products resulting from catastrophic accidents involving the mixing of hypergolic liquid rocket propellants. The analysis methods described in this report have been developed for the A-50/NTO propellant combination, but the general thermodynamic methods are applicable to any other fuel/oxidizer combination which may be encountered in an accidental hypergolic vapor release. The salient features of the computational methods described in this report are:

1. Stoichiometric reactions of A-50 fuel and NTO oxidizer have been successfully characterized using the NASA SP-273 computer program for the calculation of complex chemical equilibrium and rocket performance. Reactions have been defined according to the type of propellant accident (open-field, open-silo, closed-silo, and hypergolic explosion) and according to the presence of interacting air. For a catastrophic accident involving the full inventory of liquid oxidizer (207, 560 pounds nitrogen tetroxide) and liquid fuel (104, 609 pounds Aerozine-50) which occurs in an open Titan II missile silo, the calculated adiabatic flame temperature is 2916°K (5249°R) which is consistent with fireball data previously reported in the literature¹⁵. This calculation was performed assuming thermal interaction of air present in the closed silo ($125,000\text{ ft}^3$ air). The major gaseous combustion products contained in the fireball were determined to be carbon monoxide, carbon dioxide, hydrogen radical, hydrogen, water vapor, nitric oxide, nitrogen, hydroxide radical, and oxygen.
2. For hypergolic combustion under nonstoichiometric conditions (O/F mole ratio $\neq 1.02$) a calculation methodology is presented in which the heat evolved from the stoichiometric reaction was used to heat and vaporize the excess propellant. Major fireball components for the fuel-rich reaction were hydrazine vapor, UDMH vapor, nitrogen gas and

water vapor for accident scenarios which favored A-50 evaporation; and ammonia vapor, UDMH vapor, nitrogen gas, hydrogen gas, and water vapor for accidents characterized by A-50 evaporation and hydrazine monodecomposition. Fuel-lean hypergolic reactions contained both nitrogen dioxide gas and nitrogen tetroxide gas in the vapor phase of the fireball, the proportions of which depended upon the adiabatic temperature of the resultant fireball. Oxidizer to fuel mole ratios above 17.7 and below 0.06 were not characterized in this analysis, because the thermal energies derived from these hypergolic reactions were not sufficient to vaporize the excess propellant.

3. A generalized scheme for determining time-temperature and heat flux-temperature profiles for hypergolic fireballs is discussed. The development of the heat flux equations was based on the assumption that the major heat loss mechanism during fireball generation and lift-off was radiative, and conductive and convective heat losses were negligible. This is consistent with fireball heat transfer mechanisms previously reported in the literature²¹. The largest initial heat flux calculated was for the stoichiometric reaction of A-50 fuel and NTO oxidizer. This reaction gave an initial heat flux and temperature of 400 Btu/ft² second and 2979°K, respectively. The temperature of the fireball for this stoichiometric combustion dropped to approximately 2240°K at lift-off ($t' = 1.0$). Nonstoichiometric hypergolic combustions yielded much smaller initial heat fluxes and temperatures

($Q/A = 2.15$ Btu/ft² second, $T = 810^{\circ}\text{K}$ for $O/F = 5.1$;

$Q/A = 5.98$ Btu/ft² second, $T = 1046^{\circ}\text{K}$ for $O/F = 0.20$).

As a result, the initial adiabatic flame temperature for these nonstoichiometric hypergolic reactions did not change appreciably during fireball generation and lift-off.

4. Fireball sizes were estimated using the theoretical equations:

$$r_b = \left[\frac{3}{4\pi\rho} \right]^{1/3} W_b^{1/3}$$

Where r_b = fireball radius

W_b = total propellant weight (lbs) in reaction

ρ = density of combustion products

for an ideal gas:

$$\rho = \frac{MW_{avg} P}{RT_f}$$

Where MW_{avg} = average molecular weight of combustion gases

P = pressure of gases (14.7 psia under standard conditions)

R = Ideal gas constant (10.731 ft³ - psia/°R - mole)

T_f = adiabatic flame temperature (°R)

The calculated fireball radius for an accident involving the full inventory of A-50 fuel and NTO oxidizer ($W_b = 3.12 \times 10^5$ pound; $MW_{avg} = 21.9$; $T_f = 5249^\circ R$) using this approach is approximately 235 feet which generally corresponds to the fireball radius established empirically for A-50/NTO reactions²⁰:

$$r_b = 4.43 W_b^{0.328} = 281 \text{ feet}$$

5. Computational methods using the SP-273 computer program were used to predict the thermal energies and chemical reaction products resulting from the mixing of a hypergolic liquid rocket propellant with other chemical

species that may be encountered in a highway or rail accident. Although these calculations were performed assuming ideal thermodynamic conditions for the chemical reactants and products, they are still useful for estimating fireball temperatures and hazardous vapor envelopes for these accident scenarios.

In addition to the computational methods described above for the characterization of critical fireball parameters (e.g., chemical composition, thermal energy, and geometric size), an exhaustive literature survey was completed in order to compile existing knowledge in the hydrazine (MMH, UDMH) - nitrogen tetroxide hypergolic reaction. Over 50 chemical reaction products resulting from this combination have been described in the literature, and most of these products can be accounted for by one or more simple chemical mechanisms. One of these chemical components, nitrosodimethylamine, is of particular concern in a hypergolic bipropellant accident, because it is a confirmed product in both the A-50/NTO reaction and in the A-50/air reaction, and is a known carcinogen.

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APPENDIX A
COMPUTER OUTPUT
AEROZINE-50/NITROGEN TETROXIDE REACTIONS

Case No.	O/F Mole Ratio	Air Weight Percent	Pressure Atm	Page
1	.90	2.9	1.0	60
1	.90	2.9	12.56	61
1	.90	2.9	60.3	62
1	.90	2.9	71.9	63
2	.90	23.3	1.0	64
2	.90	23.3	12.56	65
3	.90	75.2	1.0	66
3	.90	75.2	12.56	67
4	.90	96.8	1.0	68
4	.90	96.8	12.56	69
5	.90	99.7	1.0	70
5	.90	99.7	12.56	71
5	1.02	3.1	1.0	72
6	1.02	3.1	12.56	73
6	1.02	3.1	59.0	74
6	1.02	3.1	70.6	75
19	1.02	0.0	1.0	76
19	1.02	0.0	12.56	77
32	0.51	0.0	1.0	78
20	0.20	0.0	1.0	79
21	0.10	0.0	1.0	80
23	0.01	0.0	1.0	81
33	2.0	0.0	1.0	82
26	5.1	0.0	1.0	83
28	51.0	0.0	1.0	84
30	510.0	0.0	1.0	85

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

CHEMICAL FORMULA		WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
FUEL	N 2.00000 H 4.00000	.50000	12100.000	L	298.15	0.0000
FUEL	C 2.00000 H 8.00000	.50000	11900.000	L	298.15	0.0000
OXIDANT	N 2.00000 O 4.00000	.95640	-4676.000	L	298.15	0.0000
OXIDANT	N 1.56176 O .41959	.04360	-28.200	G	298.15	0.0000

PERCENT FUEL = 32.5098 EQUIVALENCE RATIO = 1.1157 DENSITY = 0.0000

D/F = 2.0760

THERMODYNAMIC PROPERTIES

P. ATM 1.000

T. DEG K 2916

M. CAL/G 60.7

S. CAL/(G)(K) 3.0685

M. MOL WT 21.894

(DLV/DLP)T -1.03689

(DLV/DLP)P 1.7869

CP. CAL/(G)(K) 2.0254

GAMMA (S) 1.1188

CPF. CAL/(G)(K) .4782

SON VEL. M/SEC 1113.2

MOLE FRACTIONS

AR .00021

CO .07225

CO2 .04519

H .03327

H2O .00001

H2 .07615

H2O .34286

NO .00977

N2 .33634

O .01283

OH .04666

O2 .02346

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

PRODUCT	MOLE FRACTION	PRODUCT	MOLE FRACTION	PRODUCT	MOLE FRACTION
C(S)	0	CH	0	CH20	0
C2	0	C2H2	0	C2H6	0
C3	0	C4	0	HCN	0
H2O(S)	0	C3O2	0	NCN	0
N2H4	0	H2O(L)	0	NCO	0
		N2H4(L)	0	N2O4(L)	0
				N2O4	0
				N	0
				CH2	0
				C2H4	0
				C5	0
				CH	0
				C2H	0
				C4	0
				H2O2	0
				N2O	0
				CH3	0
				C2N	0
				C2H	0
				HCN	0
				NH2	0
				N3	0
				CH4	0
				C2N2	0
				HNCO	0
				NH	0
				NH3	0
				O3	0
				CN	0
				C2N2H8(L)	0
				HNCO	0
				HNCO2	0
				NO2	0
				C2N2H8	0
				HNCO3	0
				NO3	0
				CN2	0

NOTE: WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

CHEMICAL FORMULA	
FUEL N 2.00000	H 4.00000
FUEL C 2.00000	O 8.00000
OXIDANT N 2.00000	N 2.00000
OXIDANT N 1.56176	O 4.1959
AR 0.00932	C 0.00030

O/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 12.56
T. DEG K 3180
H. CAL/G 60.7
S. CAL/(G)(K) 2.8415

M. MOL WT 22.412
(DLV/DLP)T -1.02664
(DLV/DLP)P 1.5335
CP. CAL/(G)(K) 1.4477
GAMMA (S) 1.1330
CPF. CAL/(G)(K) .4824
SON VEL. M/SEC 1156.1

MOLE FRACTIONS

AR .00021
CO .06946
CO2 .05178
H .01925
H2 .00002
H2 .06655
H2O .37307
N .00001
N2 .01120
N2 .34369
O .00726
OH .04114
O2 .01634

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C4	C5	HCN	HCO	HNC	HNO	HNO2	HNO3
H2O(S)	H2O(L)	NCO	NH	NH2	NH3	NO2	NO3	N2H4
N2H4(L)	N2O	N2O4(L)	N2O5	N3	O3			

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000

FUEL C 2.00000 H 2.00000 N 2.00000

OXIDANT N 2.00000 O 4.00000

OXIDANT N 1.56176 O .41959 AR .00932 C .00030

O/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

WT FRACTION (SEE NOTE)

ENTHALPY CAL/MOL

STATE

TEMP DEG K

DENSITY G/CC

THERMODYNAMIC PROPERTIES

P. ATM 60.30

T. DEG K 3340

H. CAL/G 60.7

S. CAL/(G)(K) 2.7034

M. MOL WT 22.731

(DLV/DLP)T -1.02075

(DLV/DLP)P 1.4026

CP. CAL/(G)(K) 1.1822

GAMMA (S) 1.1425

CPF. CAL/(G)(K) .4848

SON VEL. M/SEC 1181.4

MOLE FRACTIONS

AR .00022

CO .06643

CO2 .05653

H .01261

H2O .00001

H2 .00003

H2 .05947

H2O .39304

H2O2 .00001

N .00001

NO .01131

NO2 .00001

N2 .34860

O .00450

OH .03534

O2 .01187

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C

C2 C2H

C3 C3O2

H2O(L) NCO

N2O4(L) N2O5

CH C2H2

CH2 C2H4

CH3 C2H6

CH4 C2H2

CN C2N2H8(L)

CN2 C2N2H8

CN2H4(L) HNO2

CN2H4(L) HNO3

CN2H4(L) N2O

CN2H4(L) N2O4

CN2H4(L) N2O4

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 1

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
 FUEL C 2.00000 H 8.00000 N 2.00000
 OXIDANT N 2.00000 O 4.00000
 OXIDANT N 1.56176 O .41959 AR .00932 C .00030

O/F= 2.0760 PERCENT FUEL= 32.5098 EQUIVALENCE RATIO= 1.1157 DENSITY= 0.0000

WT FRACTION
(SEE NOTE)
.50000
.50000
.95640
.04360

ENTHALPY
CAL/MOL

12100.000
11900.000
-4676.000
-28.200

STATE

L
L
L
G

TEMP
DEG K

298.15
298.15
298.15
298.15

DENSITY
G/CC

0.0000
0.0000
0.0000
0.0000

THERMODYNAMIC PROPERTIES

P. ATM 71.90
 T. DEG K 3357
 H. CAL/G 60.7
 S. CAL/(G)(K) 2.6880
 M. MOL WT 22.766
 (DLV/DLP)T -1.02012
 (DLV/DLP)P 1.3892
 CP. CAL/(G)(K) 1.1562
 GAMMA (S) 1.1436
 CPF. CAL/(G)(K) .4850
 SON VEL. M/SEC 1184.2

MOLE FRACTIONS

AR .00022
 CO .06603
 CO2 .05712
 H .01197
 HNO .00001
 H2 .00003
 H2 .05865
 H2O .528
 H2O2 .00001
 N .00001
 NH2 .00001
 NO .01127
 NO2 .00001
 N2 .34916
 O .00424
 OH .03459
 O2 .01138

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HNO2	HNO3	H2O(S)
H2O(L)	NCO	NH	NH3	NO3	N2H4	N2H4(L)	N2O	N2O4	H2O4(L)
N2O5	N3	O3							

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 2

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
 FUEL C 2.00000 H 8.00000 N 2.00000
 OXIDANT N 2.00000 O 4.00000
 OXIDANT N 1.56176 O .41959 AR .00932 C .00030

O/F= 2.8900 PERCENT FUEL= 25.7069 EQUIVALENCE RATIO= .9839 DENSITY= 0.0000

WT FRACTION (SEE NOTE) ENTHALPY CAL/MOL STATE TEMP DEG K DENSITY G/CC
 .50000 12100.000 L 298.15 0.0000
 .50000 11900.000 L 298.15 0.0000
 .68660 -4676.000 L 298.15 0.0000
 .31340 -28.200 G 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
 T. DEG K 2833
 H. CAL/G 47.8
 S. CAL/(G)(K) 2.8588
 M. MOL WT 23.624
 (DLV/DLP)T -1.02779
 (DLV/DLP)P 1.6163
 CP. CAL/(G)(K) 1.6140
 GAMMA (S) 1.1215
 CPF. CAL/(G)(K) .4414
 SON VEL. M/SEC 1057.5

MOLE FRACTIONS

AR .00177
 CO .04883
 CO2 .05228
 H .01901
 H2O .00001
 H2 .04329
 H2O .31854
 NO .01177
 N2 .41865
 O .01133
 OH .04054
 O2 .03399

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNC	HNO2	HNO3
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH3	NH2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE: WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 3

CHEMICAL FORMULA			
FUEL	N	2.00000	H 4.00000
FUEL	C	2.00000	H 8.00000
OXIDANT	N	2.00000	O 4.00000
OXIDANT	N	1.56176	O .41959
	AR	.00932	C .00030

O/F= 11.0400 PERCENT FUEL= 8.3056 EQUIVALENCE RATIO= .4503 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P, ATM 1.000

T, DEG K 1801

H, CAL/G 14.8

S, CAL/(G)(K) 2.2574

M, MOL WT 27.767

(DLV/DLP)T -1.00007

(DLV/DLP)P 1.0028

CP, CAL/(G)(K) .3504

GAMMA (S) 1.2584

CPF, CAL/(G)(K) .3336

SON VEL, M/SEC 823.7

MOLE FRACTIONS

AR .00672

CO .00002

CO2 .03857

H2 .00002

H2O .14832

N2 .00329

N2O .00001

N2 .66620

O .00004

OH .00074

O2 .13606

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH3	CH4	CN	CNH	CN2
C2	C2H	C2H2	C2H4	C2H6	C2H8	C2H2H8(L)	C2H2H8	C2O
C3	C3O2	C4	C5	H	HCO	HNC	HNO	HN2
HN2	H2O(S)	H2O(L)	H2O2	N	NC	NH	NH2	NH3
N2O	N2H4	N2H4(L)	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 3

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
 FUEL C 2.00000 H 8.00000
 OXIDANT N 2.00000 O 4.00000
 OXIDANT N 1.56176 O 4.1959

AR .00932 C .00030

O/F= 11.0400 PERCENT FUEL= 8.3056 EQUIVALENCE RATIO= .4503 DENSITY= 0.0000

WT FRACTION (SEE NOTE) .50000
 .50000
 .18000
 .82000

ENTHALPY CAL/MOL
 12100.000
 11900.000
 -4678.000
 -28.200

STATE
 L
 L
 L
 G

TEMP DEG K 298.15
 298.15
 298.15
 298.15

DENSITY G/CC
 0.0000
 0.0000
 0.0000
 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 12.56
 T. DEG K 1803
 H. CAL/G 14.8
 S. CAL/(G)(K) 2.0763
 M. MOL WT 27.771
 (DLV/DLP)T -1.00004
 (DLV/DLP)P 1.0013
 CP. CAL/(G)(K) .3461
 GAMMA (S) 1.2614
 CPF. CAL/(G)(K) .3336
 SON VEL. M/SEC 825.0

MOLE FRACTIONS

AR .00672
 CO .00001
 CO2 .03859
 H2 .00001
 H2O .14853
 NO .00331
 NO2 .00002
 N2 .66827
 O .00001
 OH .00040
 O2 .13613

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C
 C2 C2H
 C3 C3O2
 HNO3 H2O
 NO3 N2H4
 CH CH2
 C2H2 C2H4
 C4 C5
 H2O(S) H2O(L)
 N2H4(L) N2O
 CH2O C2H6
 C2H4 H
 H2O2 H2O4
 N2O4 N2O4(L)
 CH3 C2H
 C2H2 HCN
 N N2O4(L)
 CH4 C2H2
 HCO HCO
 NCO N2O5
 CN C2H2H8(L)
 HNCO HNO
 NH NH2
 N3 O3
 CHN C2H2H8
 HNO HNO2
 NH2 NH3
 O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 4

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
 FUEL C 2.00000 H 8.00000 N 2.00000
 OXIDANT N 2.00000 O 4.00000
 OXIDANT N 1.56176 O .41959 AR .00932 C .00030

O/F= 92.5700 PERCENT FUEL= 1.0687 EQUIVALENCE RATIO= .0713 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
 T. DEG K 536
 H. CAL/G 1.1
 S. CAL/(G)(K) 1.7998
 M. MOL WT 28.805
 (DLV/DLP)T -1.00000
 (DLV/DLT)P 1.0000
 CP. CAL/(G)(K) .2507
 GAMMA (S) 1.3796
 CPF. CAL/(G)(K) .2507
 SON VEL. M/SEC 462.1

MOLE FRACTIONS

AR .00898
 CO2 .00541
 H2O .01985
 N2 .76584
 O2 .19992

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH3	CH4	CN	CN2	C2N2H8
CO	C2	C2H	C2H2	C2H6	C2N	C2N2H8(L)	C2N2H8	
C2O	C3	C3O2	C4	H	H2O2	H2CO	H2O	
H2O2	H2O3	H2O	H2	H2O(L)	N2O2	N	NH	
NH2	NH3	NO	NO2	N2H4	N2H4(L)	N2O	N2O4	
N2O5	N3	O	OH	O3				N2O4(L)

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

CASE NO. 4

FUEL	N	2.00000	H	4.00000
FUEL	C	2.00000	H	8.00000
OXIDANT	N	2.00000	O	4.00000
OXIDANT	N	1.56176	O	.41959

WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
.50000	12100.000	L	298.15	0.0000
.50000	11900.000	L	298.15	0.0000
.02140	-4676.000	L	298.15	0.0000
.97860	-28.200	G	298.15	0.0000

D/F= 92.5700 PERCENT FUEL= 1.0687 EQUIVALENCE RATIO= .0713 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM	12.56
T. DEG K	536
H. CAL/G	1.1
S. CAL/(G)(K)	1.6253
M. MOL WT	28.805
(DLV/DLP)T	-1.00000
(DLV/DLT)P	1.0000
CP. CAL/(G)(K)	.2507
GAMMA (S)	1.3796
CPF.CAL/(G)(K)	.2507
SON VEL. M/SEC	462.1

MOLE FRACTIONS

AR	.00898
C02	.00541
420	.01985
42	.76584
22	.19992

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	C(S)	CH	CH2	CH2O	CH3	CH4	CN	CHN	CH2
C2	C2O	C2H	C2H2	C2H4	C2H6	C2H8	C2H2	C2H2H8	C2H2H8 (L)
C3	C3O	C3O2	C4	C5	H	HCN	HCO	HNC	H4O
H#O3	H#O2	H#O2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
H#3	H#2	NO	NO2	O3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N3	H2O5	O	OH						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 5

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000
OXIDANT N 2.00000 O 4.00000
OXIDANT N 1.56176 O .41959

O/F=907.8000 PERCENT FUEL= .1100 EQUIVALENCE RATIO= .0088 DENSITY= 0.0000

WT FRACTION (SEE NOTE) ENTHALPY CAL/MOL STATE TEMP DEG K DENSITY G/CC
.50000 12100.000 L 298.15 0.0000
.50000 11900.000 L 298.15 0.0000
.00220 -4676.000 L 298.15 0.0000
.99780 -28.200 G 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 323
H. CAL/G -8
S. CAL/(G)(K) 1.6612
M. MOL WT 28.948
(DLV/DLP)T -1.00000
(DLV/DLP)P 1.0000
CP. CAL/(G)(K) .2407
GAMMA (S) 1.3991
CPF. CAL/(G)(K) .2407
SON VEL. M/SEC 360.4

MOLE FRACTIONS

AR .00929
CO2 .00083
H2O .00205
N2 .77932
O2 .20851

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HACO	HNO
HNO2	HNO3	H2O2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 5

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000
OXIDANT N 2.00000 O 4.00000
OXIDANT N 1.56176 O .41959

O/F=907.8000 PERCENT FUEL= .1100 EQUIVALENCE RATIO= .0088 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 12.56
T. DEG K 323
H. CAL/G -.8
S. CAL/(G)(K) 1.4874
M. MOL WT 28.948
(DLV/DLP)T -1.00000
(DLV/DLP)P 1.0000
CP. CAL/(G)(K) .2407
GAMMA (S) 1.3991
CPF. CAL/(G)(K) .2407
SON VEL. M/SEC 360.4

MOLE FRACTIONS

AR .00929
CO2 .00083
H2O .00205
N2 .77932
O2 .20851

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	CN	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCN	HNC	HNO
HNO2	HNO3	H2O2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000
OXIDANT N 2.00000 O 4.00000
OXIDANT N 1.56176 O .41959

N 2.00000

AR .00332 C .00030

O/F= 2.3480

PERCENT FUEL= 29.8686

EQUIVALENCE RATIO=

.9864

DENSITY= 0.0000

WT FRACTION
(SEE NOTE)

ENTHALPY
CAL/MOL

STATE

TEMP
DEG K

DENSITY
G/CC

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2907
H. CAL/G 51.8
S. CAL/(G)(K) 2.9872
M. MOL WT 22.682
(DLV/DLP) T -1.03672
(DLV/DLP) P 1.7883
CP. CAL/(G)(K) 1.9736
GAMMA (S) 1.1176
CPF. CAL/(G)(K) .4638
SON VEL. M/SEC 1091.3

MOLE FRACTIONS

AR .00022
CO .05996
CO2 .05277
H .02746
H2 .00001
H2O .05527
NO .34162
N2 .01286
O .33967
OH .01643
O2 .05245
O2 .04126

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C
C2 C2H
C3 C3O2
H2O(S) H2O(L)
N2H4 N2H4(L)

CH
C2H2
C4
H2O2
N2O

CH2
C2H4
C5
N
N2O4
N2O4(L)

CH3
C2N
HCN
NH
N2O5

CH4
C2N2
HNC
NH2
N3

CN
C2N2HB(L)
HNO
NH3
O3

CN2
C2O
HNO3
NO3

NOTE: WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
 FUEL C 2.00000 H 8.00000
 OXIDANT N 2.00000 O 4.00000
 OXIDANT N 1.56176 O .41959 AR .00932 C .00030

WT FRACTION (SEE NOTE)
 .50000
 .50000
 .95640
 .04360

ENTHALPY CAL/MOL
 12100.000
 11900.000
 -4676.000
 -28.200

STATE
 L
 L
 L
 G

TEMP DEG K
 298.15
 298.15
 298.15
 298.15

DENSITY G/CC
 0.0000
 0.0000
 0.0000
 0.0000

O/F = 2.3480 PERCENT FUEL = 29.8686 EQUIVALENCE RATIO = .9864 DENSITY = 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 12.56
 T. DEG K 3168
 H. CAL/G 51.8
 S. CAL/(G)(K) 2.7681

M. MOL WT 23.220
 (DLV/DLP)T -1.02715
 (DLV/DLP)P 1.5466
 CP. CAL/(G)(K) 1.4317
 GAMMA (S) 1.1310
 CPF. CAL/(G)(K) .4679
 SON VEL. M/SEC 1132.7

MOLE FRACTIONS

AR .00023
 CO .05480
 CO2 .06060
 H .01527
 HNO .00001
 H2 .00003
 H2 .04472
 H2O .37090
 H2O2 .00001
 N .00001
 NO .01585
 NO2 .00001
 N2 .34638
 O .01000
 OH .04790
 O2 .03330

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C CH CH2 CH2O CH3 CH4 CN C2N2H8(L) CNH C2N2H8 C2O
 C2 C2H C2H2 C2H6 C2N C2N2H8(L) C2N2H8 C2N2H8
 C3 C302 C4 C5 HCN HCO HCO3 H2O(S) H2O4
 H2O(L) NH NH2 NH3 NH4 N2O N2O4
 N2O4(L) N2O5 N3

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
 FUEL C 2.00000 H 8.00000 N 2.00000
 OXIDANT N 2.00000 O 4.00000
 OXIDANT N 1.56176 O .41959 AR .00932 C .00030

O/F= 2.3480 PERCENT FUEL= 29.8686 EQUIVALENCE RATIO= .9864 DENSITY= 0.0000

WT FRACTION (SEE NOTE) ENTHALPY CAL/MOL STATE TEMP DEG K DENSITY G/CC
 .50000 12100.000 L 298.15 0.0000
 .50000 11900.000 L 298.15 0.0000
 .95640 -4676.000 L 298.15 0.0000
 .04360 -28.200 G 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 59.00
 T. DEG K 3326
 H. CAL/G 51.8
 S. CAL/(G)(K) 2.6366
 M. MOL WT 23.552
 (DLV/DLP)T -1.02189
 (DLV/DLT)P 1.4260
 CP. CAL/(G)(K) 1.1890
 GAMMA (S) 1.1395
 CPF. CAL/(G)(K) .4703
 SON VEL. M/SEC 1156.7

MOLE FRACTIONS

AR .00023
 CO .04988
 CO2 .06718
 H .00976
 H2O .00001
 H2 .00005
 H2 .03737
 H2O .38989
 H2O2 .00001
 N .00001
 NO .01721
 NO2 .00002
 N2 .35075
 O .00673
 OH .04283
 O2 .02804

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C3	C3O2	C3	C5	HCN	HCD	HNC	HN2	HN2(S)
H2O(L)	NCO	NH	NH2	NH3	N2O	N2H4	N2H4(L)	N2O4
N2O4(L)	N2O5	N3	O3					

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 6

CHEMICAL FORMULA				WT FRACTION	ENTHALPY	STATE	TEMP	DENSITY
				(SEE NOTE)	CAL/MOL		DEG K	G/CC
FUEL	N	2.00000	H	4.00000	12100.000	L	298.15	0.0000
FUEL	C	2.00000	H	8.00000	11900.000	L	298.15	0.0000
OXIDANT	N	2.00000	O	4.00000	-4676.000	L	298.15	0.0000
OXIDANT	N	1.56176	O	.41959	-28.200	G	298.15	0.0000

O/F = 2.3480 PERCENT FUEL = 29.8686 EQUIVALENCE RATIO = .9864 DENSITY = 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 70.60
T. DEG K 3344
H. CAL/G 51.8
S. CAL/(G)(K) 2.6215
M. MOL WT 23.590
(DLV/DLP)T -1.02131
(DLV/DLP)P 1.4133
CP. CAL/(G)(K) 1.1697
GAMMA (S) 1.1405
CPF. CAL/(G)(K) .4706
S. VEL. M/SEC 1159.4

FUEL FRACTIONS

AR .00023
CO .04922
CG2 .06802
H .00923
HNO .00001
H2 .00006
H2O .03650
H2O .39210
H2O2 .00002
N .00001
NO .01733
NO2 .00002
N2 .35127
N2O .00001
O .00640
OH .04215
O2 .02742

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNV	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNCO	HN2	HN2O3	H2O(S)
H2O(L)	NCO	NH	NH2	NH3	NO3	N2H4	N2H4(L)	N2O4	N2O4(L)
N2O5	NO	O3							

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 19

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F= 2.2450 PERCENT FUEL= 30.8166 EQUIVALENCE RATIO= 1.0017 DENSITY= 0.0000

WT FRACTION
(SEE NOTE)
.50000
.50000
1.00000

ENTHALPY
CAL/MOL
12100.000
11900.000
-4675.000

STATE
L
L
L

TEMP
DEG K
298.15
298.15
298.15

DENSITY
G/CC
0.0000
0.0000
0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2918
H. CAL/G 53.5
S. CAL/(G)(K) 3.0162
M. MOL WT 22.448
(DLV/DLP) T 1.03828
(DLV/DLP) P 1.5176
CP. CAL/(G)(K) 2.0417
GAMMA (S) 1.1173
CPF. CAL/(G)(K) .4689
SON VEL. M/SEC 1098.9

MOLE FRACTIONS

CO .06301
CO2 .05210
H .02952
H2 .00001
H2O .05926
NO .34523
NO2 .01260
N2 .3273
O .01.82
OH .05366
O2 .03980

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C
C2 C2H
C3 C3O2
H2O(S) 1/2 O2(L)
N2H4 N2H4(L)
C2H2 C2H2
C4 C4
H2O2 H2O2
N2O N2O
C2H4 C2H4
C2H6 C2H6
HCN HCN
NCD NCD
N2O4(L) N2O4(L)
N2O4 N2O4
N N
NH NH
N2 N2
N3 N3
CH3 CH3
C2N C2N
HCO HCO
NH2 NH2
N2O5 N2O5
CH4 CH4
C2N2 C2N2
HNC HNC
NH3 NH3
O3 O3
CN CN
C2N2H8(L) C2N2H8
HNO2 HNO2
NO2 NO2
C2N C2N
C2N2H8 C2N2H8
HNO3 HNO3
NO3 NO3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 19

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F = 2.2350 PERCENT FUEL = 30.8166 EQUIVALENCE RATIO = 1.0017 DENSITY = 0.0000

WT FRACTION (SEE NOTE) ENTHALPY CAL/MOL STATE TEMP DEG K DENSITY G/CC
.50000 12100.000 L 298.15 0.0000
.50000 11900.000 L 298.15 0.0000
1.00000 -4676.000 L 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 12.56
T. DEG K 3185
H. CAL/G 53.5
S. CAL/(G)(K) 2.7949
M. MOL WT 22.993
(DLV/DLP)T -1.02844
(DLV/DLT)P 1.5687
CP. CAL/(G)(K) 1.4782
GAMMA (S) 1.1305
CPF. CAL/(G)(K) .4731
SON VEL. M/SEC 1141.0

MOLE FRACTIONS

CO .05825
CO₂ .05965
H .01668
H₂O .00001
H₂ .00003
H₂ .04868
H₂O .37526
H₂O .00001
N .00001
NO .01551
NO₂ .00001
N₂ .33462
O .01028
OH .04320
O₂ .03182

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C C₂H C₂H₂ CH₂ CH₂O CH₃ CH₄ CN C₂N₂H₈(L) CN₂
C₂ C₂H C₂H₂ C₂H₄ C₂H₆ C₂N C₂N₂H₈(L) C₂N₂H₈
C₃ C₃O₂ C₄ C₅ HCN HCO HNO₃ HNO₂ H₂O(S) C₂O
H₂O(L) NCO NH₂ NH₃ N₂H₄ N₂O N₂O₄
N₂O₄(L) N₂O₅ O₃

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUEL AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 32

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F= 1.1220

PERCENT FUEL= 47.1254

EQUIVALENCE RATIO= 2.0043

DENSITY= 0.0000

WT FRACTION (SEE NOTE) 50000 50000 1.00000
ENTHALPY CAL/MOL 12100.000 11900.000 -4676.000
STATE L L L
TEMP DEG K 298.15 298.15 298.15
DENSITY G/CC 0.0000 0.0000 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2603
H. CAL/G 108.8
S. CAL/(G)(K) 3.4772
M. MOL WT 17.868
(DLV/DLP)T -1.00650
(DLV/DLP)P 1.1448
CP. CAL/(G)(K) .9134
GAMMA (S) 1.1807
CPS. CAL/(G)(K) .5492
SUN VEL. M/SEC 1195.9

MOLE FRACTIONS

CO .12301
CO2 .01710
H .02051
H2 .28198
H2O .24865
NO .00033
N2 .30395
C .00020
OH .00418
O2 .00007

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C CH CH2 CH3 CH4 CN CN2 CN2H8
C2 C2H C2H2 C2H4 C2H6 C2N C2N2H8(L)
C3 C302 C4 C5 HCN HCO HNO2
H2O H2O(S) H2O(L) H2O2 N NCO N2O4(L)
NO3 N2H4 N2H4(L) N2O N205 N3 NH3 NO2

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 20

CHEMICAL FORMULA

FUEL	W	2.00000	I	4.00000
FUEL	C	2.00000	H	3.00000
O ₂ IDANT	N	2.00000	O	4.00000

N 2.00000

D/F= .4490 PERCENT FUEL= 69.0131 EQUIVALENCE RATIO= 5.0085 DENSITY= 0.0000

WT FRACTION (SEE NOTE)

ENTHALPY	STATE	TEMP	DENSITY
CAL/MOL		DEG K	G/CC
12100.000	L	298.15	0.0000
11900.000	L	298.15	0.0000
-4676.000	L	298.15	0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000

T. DEG K 1372

H. CAL/G 182.9

S. CAL/(G)(K) 3.8696

M. MOL WT 13.183

(DLV/DLP)T -1.00013

(DLV/DLP)P 1.0012

CP. CAL/(G)(K) .6087

GAMMA (S) 1.3300

GPF. CAL/(G)(K) .6038

SON VEL. M/SEC 1072.8

MOLE FRACTIONS

CH4 .00003

CO .14835

CO2 .00300

H2 .56334

H2O .02323

NH3 .00002

N2 .26203

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2
C2H	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8(L)	C2N2H8	C2O	C3
C3O2	C4	H	H2O2	H2O	H2CO	H2CO	HNO	HNO2	HNO3
H2O	H2O(S)	H2O(L)	N	N2O	N2O4(L)	NH	NH2	NO	NO2
NO3	N2H4	N2H4(L)	N2O4	N2O4(L)	N2O5	N2O5	N3	O	OH
O2	O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 21

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F = .2245 PERCENT FUEL = 81.6660 EQUIVALENCE RATIO = 10.0169 DENSITY = 0.0000

THERMODYNAMIC PROPERTIES

P, ATM 1.000
T, DEG K 1086
H, CAL/G 225.7
S, CAL/(G)(K) 3.8981
M, MOL WT 12.452
(DLV/DLP)T -1.02078
(DLV/DLP)P 1.2432
Cp, CAL/(G)(K) 1.1252
GAMMA (S) 1.2475
CPF, CAL/(G)(K) .6466
SON VEL, M/SEC 950.9

MOLE FRACTIONS

C(S) .05777
CH4 .01488
CO .08586
CO2 .00090
HCN .00001
H2 .58210
H2O .00585
NH3 .00008
N2 .25254

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C302
C4	C5	H	HCO	H2CO	H2O	H2O2	HNO3	H2O(S)
H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	N2H4
N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 23

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F= .0225 PERCENT FUEL= 97.8043 EQUIVALENCE RATIO= ***** DENSITY= 0.0000

WT FRACTION (SEE NOTE) ENTHALPY CAL/MOL STATE TEMP DEG K DENSITY G/CC
.50000 12100.000 L 298.15 0.0000
.50000 11900.000 L 298.15 0.0000
1.00000 -4676.000 L 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 946
H. CAL/G 280.4
S. CAL/(G)(K) 3.8767
M. MOL WT 12.275
(DLV/DLP)T -1.05380
(OLV/DLP)P 1.6248
CP. CAL/(G)(K) 1.8952
GAMMA (S) 1.2073
GPF. CAL/(G)(K) .7043
SON VEL. M/SEC 879.3

MOLE FRACTIONS

C(S) .10830
CH4 .06349
CO .00626
CO2 .00008
H2 .55903
H2O .00402
NH3 .00020
N2 .25861

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C302
C4	C5	H	HCN	HCO	HNC	HNO	HNO2	HNO3	H2
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH	O2
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 33

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

WT FRACTION (SEE NOTE)
ENTHALPY CAL/MOL
STATE
TEMP DEG K
DENSITY G/CC

O/F= 4.4900 PERCENT FUEL= 18.2149 EQUIVALENCE RATIO= .5008 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2636
H. CAL/G 10.9
S. CAL/(G)(K) 2.6006
M. MOL WT 26.375
(DLV/DLP)T -1.01134
(DLV/DLP)P 1.2783
CP. CAL/(G)(K) .9427
GAMMA (S) 1.1354
CPF. CAL/(G)(K) .3967
SON VEL. M/SEC 971.3

MOLE FRACTIONS

CO .01068
CO2 .06925
H .00364
H2O .00002
H2 .00680
H2O 28304
NO .02016
NO2 .00001
N2 .33927
O .01270
OH .03626
O2 .21816

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C CH C2H2 C2H4 C2H6 C2N CH3 CH4 C2N2H8(L) CN C2N2
C2 C2H C3O2 C4 H2O2 N2O4(L) N2O5 N3 NH3 HNO2 HNO3
C3 H2O(S) H2O(L) N2O N2H4(L) N2O

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 26

CHEMICAL FORMULA
FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

WT FRACTION (SEE NOTE)
.50000
.50000
1.00000
ENTHALPY CAL/MOL
12100.000
11900.000
-4676.000
STATE
L
L
L
TEMP DEG K
298.15
298.15
298.15
DENSITY G/CC
0.0000
0.0000
0.0000

O/F= 11.2300 PERCENT FUEL= 8.1766 EQUIVALENCE RATIO= .2002 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 1693
H. CAL/G -23.1
S. CAL/(G)(K) 2.2030
M. MOL WT 28.955
(DLV/DLP)T -1.00004
(DLV/DLP)P 1.0318
CP. CAL/(G)(K) .3368
GAMMA (S) 1.2570
CPF. CAL/(G)(K) .3229
SON VEL. M/SEC 781.6

MOLE FRACTIONS

CO2 .03939
H2O .15241
NO .00296
NO2 .00001
N2 .34411
O .00003
OH .00051
O2 .46057

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNC	HNO
HNO2	HNO3	H2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	N2	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 28

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F=112.3000 PERCENT FUEL= .8826 EQUIVALENCE RATIO= .0200 DENSITY= 0.0000

WT FRACTION (SEE NOTE) ENTHALPY CAL./MOL STATE TEMP DEG K DENSITY G/CC
.50000 12100.000 L 298.15 0.0000
.50000 11900.000 L 298.15 0.0000
1.00000 -4676.000 L 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 293
H. CAL/G -47.8
S. CAL/(G)(K) 1.6153
M. MOL WT 30.476
(DLV/DLP)T -1.00000
(DLV/DLP)P 1.0000
CP. CAL/(G)(K) .2303
GAMMA (S) 1.3950
CPF. CAL/(G)(K) .2303
SON VEL. M/SEC 334.1

MOLE FRACTIONS

CO2 .00448
H2O .01735
N2 .33473
O2 .64345

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNN	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNO	HNO
HNO2	HNO3	H2O2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH
NH2	NH3	NO	NO2	NO3	N2H4(L)	N2H4(L)	N2O	N2O4	N2O4(L)
N2O5	N3	O	OH	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 30

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT N 2.00000 O 4.00000

O/F=***** PERCENT FUEL= .0890 EQUIVALENCE RATIO= .0020 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 97
H. CAL/G -50.5
S. CAL/(G)(K) 1.3495
M. MOL WT 30.651
(DLV/DLP)T -1.00001
(DLV/DLP)P 1.0001
CP. CAL/(G)(K) .2289
GAMMA (S) 1.3952
CPF. CAL/(G)(K) .2288
SON VEL. M/SEC 191.2

MOLE FRACTIONS

CO2 .00045
HNO3 .00001
H2O .00176
N2 .33347
O2 .66431

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CN2	CN2
CO	C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8
C2O	C3	C3O2	C4	C5	H	HCN	HCO	HNC	HNC
HNO2	H2	H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2
H2O3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5
N3	O	OH	O3						

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

APPENDIX B
THERMOCHEMICAL CALCULATIONS FOR NONSTOICHIOMETRIC
COMBUSTION OF AEROZINE-50 AND NITROGEN TETROXIDE

Analysis No.	O/F Mole Ratio	Percent Mixing	Vaporization Conditions	Page
1	1.02	100	No Excess Propellant	87
2	0.51	100	H & UDMH Evaporated	88
3	0.51	100	UDMH Evaporated	89
4	0.51	100	UDMH Evaporated & H Decomp.	90
5	0.20	100	H & UDMH Evaporated	91
6	0.20	100	UDMH Evaporated & H Decomp.	92
7	0.10	100	H & UDMH Evaporated	93
8	0.10	100	UDMH Evaporated & H Decomp.	94
9	0.06	100	H & UDMH Evaporated	95
10	0.06	80	H & UDMH Evaporated	96
11	0.06	60	H & UDMH Evaporated	97
12	0.06	40	H & UDMH Evaporated	98
13	0.06	20	H & UDMH Evaporated	99
14	2.04	100	NO ₂ (g)	100
15	5.10	100	NO ₂ (g)	101
16	7.00	100	NO ₂ (g)	102
17	7.00	80	NO ₂ (g)	103
18	7.00	60	NO ₂ (g)	104
19	7.00	40	NO ₂ (g)	105
20	7.00	20	NO ₂ (g)	106
21	8.55	100	N ₂ O ₄ (g) + NO ₂ (g)	107
22	13.02	100	N ₂ O ₄ (g) + NO ₂ (g)	108
23	17.72	100	N ₂ O ₄ (g) + NO ₂ (g)	109

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 1

OXIDIZER/FUEL MOLE RATIO 1.02

PERCENT MIXING 100

VAPORIZATION CONDITIONS No Excess Propellant

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a ₁₃ = <u>0</u>	a ₁₄ = <u>0</u>	a ₁₅ = <u>0</u>
a ₁₆ = <u>0</u>	a ₁₇ = <u>0</u>	a ₁₈ = <u>0</u>
a ₁₉ = <u>0</u>		

RESULTS:

Flame Temperature 2979 OK (5363 OR)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.061
carbon dioxide	CO ₂	.050
hydrogen radical	H	.028
hydrogen	H ₂	.057
water vapor	H ₂ O	.332
nitric oxide	NO	.012
nitrogen	N ₂	.316
hydroxide	OH	.052
oxygen	O ₂	.094
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 23.13 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 2OXIDIZER/FUEL MOLE RATIO 0.51PERCENT MIXING 100VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ <u>.6545</u>	$a_{14} =$ <u>.3489</u>	$a_{15} =$ <u>0</u>
$a_{16} =$ <u>0</u>	$a_{17} =$ <u>0</u>	$a_{18} =$ <u>0</u>
$a_{19} =$ <u>0</u>		

RESULTS:Flame Temperature 1975 °K (3556 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.052
carbon dioxide	CO ₂	.043
hydrogen radical	H	.024
hydrogen	H ₂	.049
water vapor	H ₂ O	.286
nitric oxide	NO	.010
nitrogen	N ₂	.272
hydroxide	OH	.045
oxygen	O ₂	.081
hydrazine vapor	N ₂ H ₄ (g)	.090
UDMH vapor	C ₂ H ₈ N ₂ (g)	.048
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 25.66 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 3

OXIDIZER/FUEL MOLE RATIO .51

PERCENT MIXING 100

VAPORIZATION CONDITIONS UDMH Selective Evaporation

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a ₁₃ = <u>0</u>	a ₁₄ = <u>.3489</u>	a ₁₅ = <u>0</u>
a ₁₆ = <u>0</u>	a ₁₇ = <u>0</u>	a ₁₈ = <u>0</u>
a ₁₉ = <u>0</u>		

RESULTS:

Flame Temperature 2402 OK (4324 OR)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.057
carbon dioxide	CO ₂	.047
hydrogen radical	H	.026
hydrogen	H ₂	.054
water vapor	H ₂ O	.314
nitric oxide	NO	.011
nitrogen	N ₂	.299
hydroxide	OH	.049
oxygen	O ₂	.089
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.053
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 25.02 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 4OXIDIZER/FUEL MOLE RATIO .51PERCENT MIXING 100VAPORIZATION CONDITIONS UDMH Evaporation & Hydrazine Decomposition

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ <u>0</u>	$a_{14} =$ <u>.3489</u>	$a_{15} =$ <u>0</u>
$a_{16} =$ <u>.6545</u>	$a_{17} =$ <u>.3272</u>	$a_{18} =$ <u>.3272</u>
$a_{19} =$ <u>0</u>		

RESULTS:Flame Temperature 2239 °K (4031 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.048
carbon dioxide	CO ₂	.040
hydrogen radical	H	.022
hydrogen	H ₂	.086
water vapor	H ₂ O	.263
nitric oxide	NO	.009
nitrogen	N ₂	.291
hydroxide	OH	.041
oxygen	O ₂	.074
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.044
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.082
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 23.55 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 5OXIDIZER/FUEL MOLE RATIO .204PERCENT MIXING 100VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ <u>2.614</u>	$a_{14} =$ <u>1.394</u>	$a_{15} =$ <u>0</u>
$a_{16} =$ <u>0</u>	$a_{17} =$ <u>0</u>	$a_{18} =$ <u>0</u>
$a_{19} =$ <u>0</u>		

RESULTS:Flame Temperature 1046 °K (1882 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.037
carbon dioxide	CO ₂	.031
hydrogen radical	H	.017
hydrogen	H ₂	.035
water vapor	H ₂ O	.203
nitric oxide	NO	.007
nitrogen	N ₂	.193
hydroxide	OH	.032
oxygen	O ₂	.057
hydrazine vapor	N ₂ H ₄ (g)	.254
UDMH vapor	C ₂ H ₈ N ₂ (g)	.135
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 30.38 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 6OXIDIZER/FUEL MOLE RATIO .204PERCENT MIXING 100VAPORIZATION CONDITIONS UDMH Evaporation & Hydrazine Decomposition

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ <u>0</u>	$a_{14} =$ <u>1.394</u>	$a_{15} =$ <u>0</u>
$a_{16} =$ <u>2.614</u>	$a_{17} =$ <u>1.307</u>	$a_{18} =$ <u>1.307</u>
$a_{19} =$ <u>0</u>		

RESULTS:Flame Temperature 1523 °K (2742 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.029
carbon dioxide	CO ₂	.024
hydrogen radical	H	.014
hydrogen	H ₂	.129
water vapor	H ₂ O	.162
nitric oxide	NO	.006
nitrogen	N ₂	.255
hydroxide	OH	.025
oxygen	O ₂	.046
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.108
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.202
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 24.20 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 7OXIDIZER/FUEL MOLE RATIO .102PERCENT MIXING 100VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} = \underline{5.881}$ $a_{14} = \underline{3.136}$ $a_{15} = \underline{0}$
 $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$
 $a_{19} = \underline{0}$

RESULTS:Flame Temperature 580 °K (1045 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.025
carbon dioxide	CO ₂	.021
hydrogen radical	H	.011
hydrogen	H ₂	.023
water vapor	H ₂ O	.136
nitric oxide	NO	.005
nitrogen	N ₂	.130
hydroxide	OH	.021
oxygen	O ₂	.039
hydrazine vapor	N ₂ H ₄ (g)	.384
UDMH vapor	C ₂ H ₈ N ₂ (g)	.205
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 34.06 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 8OXIDIZER/FUEL MOLE RATIO .102PERCENT MIXING 100VAPORIZATION CONDITIONS UDMH Evaporation & Hydrazine Decomposition

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$	<u>0</u>	$a_{14} =$	<u>3.136</u>	$a_{15} =$	<u>0</u>
$a_{16} =$	<u>5.881</u>	$a_{17} =$	<u>2.941</u>	$a_{18} =$	<u>2.941</u>
$a_{19} =$	<u>0</u>				

RESULTS:Flame Temperature 1206 °K (2171 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.018
carbon dioxide	CO ₂	.015
hydrogen radical	H	.008
hydrogen	H ₂	.156
water vapor	H ₂ O	.098
nitric oxide	NO	.003
nitrogen	N ₂	.232
hydroxide	OH	.015
oxygen	O ₂	.028
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.148
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.278
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 24.61 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 9OXIDIZER/FUEL MOLE RATIO .060PERCENT MIXING 100VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

 $a_{13} = \underline{10.39}$ $a_{14} = \underline{5.54}$ $a_{15} = \underline{0}$ $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$ $a_{19} = \underline{0}$ RESULTS:Flame Temperature 298 °K (537 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.017
carbon dioxide	CO ₂	.014
hydrogen radical	H	.008
hydrogen	H ₂	.016
water vapor	H ₂ O	.094
nitric oxide	NO	.003
nitrogen	N ₂	.089
hydroxide	OH	.015
oxygen	O ₂	.027
hydrazine vapor	N ₂ H ₄ (g)	.468
UDMH vapor	C ₂ H ₈ N ₂ (g)	.249
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 36.49 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 10OXIDIZER/FUEL MOLE RATIO .060PERCENT MIXING 80VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} = \underline{8.31}$ $a_{14} = \underline{4.43}$ $a_{15} = \underline{0}$
 $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$
 $a_{19} = \underline{0}$

RESULTS:Flame Temperature 406 °K (731 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.020
carbon dioxide	CO ₂	.017
hydrogen radical	H	.009
hydrogen	H ₂	.019
water vapor	H ₂ O	.110
nitric oxide	NO	.004
nitrogen	N ₂	.104
hydroxide	OH	.017
oxygen	O ₂	.031
hydrazine vapor	N ₂ H ₄ (g)	.437
UDMH vapor	C ₂ H ₈ N ₂ (g)	.233
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 35.86 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 11OXIDIZER/FUEL MOLE RATIO .060PERCENT MIXING 60VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

 $a_{13} = \underline{6.23}$ $a_{14} = \underline{3.32}$ $a_{15} = \underline{0}$ $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$ $a_{19} = \underline{0}$ RESULTS:Flame Temperature 550 °K (991 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.024
carbon dioxide	CO ₂	.020
hydrogen radical	H	.011
hydrogen	H ₂	.023
water vapor	H ₂ O	.132
nitric oxide	NO	.005
nitrogen	N ₂	.125
hydroxide	OH	.021
oxygen	O ₂	.037
hydrazine vapor	N ₂ H ₄ (g)	.393
UDMH vapor	C ₂ H ₈ N ₂ (g)	.210
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 34.39 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 12OXIDIZER/FUEL MOLE RATIO .060PERCENT MIXING 40VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

 $a_{13} = \underline{4.16}$ $a_{14} = \underline{2.22}$ $a_{15} = \underline{0}$ $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$ $a_{19} = \underline{0}$ RESULTS:Flame Temperature 769 °K (1385 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.030
carbon dioxide	CO ₂	.025
hydrogen radical	H	.014
hydrogen	H ₂	.028
water vapor	H ₂ O	.166
nitric oxide	NO	.006
nitrogen	N ₂	.157
hydroxide	OH	.026
oxygen	O ₂	.047
hydrazine vapor	N ₂ H ₄ (g)	.328
UDMH vapor	C ₂ H ₈ N ₂ (g)	.176
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 32.62 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 13OXIDIZER/FUEL MOLE RATIO .060PERCENT MIXING 20VAPORIZATION CONDITIONS All Excess Hydrazine & UDMH Evaporated

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} = \underline{2.08}$ $a_{14} = \underline{1.11}$ $a_{15} = \underline{0}$
 $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$
 $a_{19} = \underline{0}$

RESULTS:Flame Temperature 1202 °K (2164 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.040
carbon dioxide	CO ₂	.033
hydrogen radical	H	.019
hydrogen	H ₂	.038
water vapor	H ₂ O	.220
nitric oxide	NO	.008
nitrogen	N ₂	.209
hydroxide	OH	.034
oxygen	O ₂	.062
hydrazine vapor	N ₂ H ₄ (g)	.219
UDMH vapor	C ₂ H ₈ N ₂ (g)	.117
nitrogen dioxide	NO ₂	.000
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 29.33 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 14OXIDIZER/FUEL MOLE RATIO 2.04PERCENT MIXING 100VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 1.02
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$ 0

RESULTS:Flame Temperature 1958 °K (3525 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.046
carbon dioxide	CO ₂	.038
hydrogen radical	H	.021
hydrogen	H ₂	.043
water vapor	H ₂ O	.251
nitric oxide	NO	.009
nitrogen	N ₂	.238
hydroxide	OH	.039
oxygen	O ₂	.071
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.245
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 28.72 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 15OXIDIZER/FUEL MOLE RATIO 5.1PERCENT MIXING 100VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 4.0783
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$ 0

RESULTS:Flame Temperature 810 °K (1459 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.026
carbon dioxide	CO ₂	.022
hydrogen radical	H	.012
hydrogen	H ₂	.025
water vapor	H ₂ O	.144
nitric oxide	NO	.005
nitrogen	N ₂	.137
hydroxide	OH	.022
oxygen	O ₂	.041
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.565
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 36.01 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 16

OXIDIZER/FUEL MOLE RATIO 7.00

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N₂O₄ (l) 100% Dissociated into NO₂ (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

a₁₃ = 0 a₁₄ = 0 a₁₅ = 5.98
a₁₆ = 0 a₁₇ = 0 a₁₈ = 0
a₁₉ = 0

RESULTS:

Flame Temperature 486 °K (875 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.021
carbon dioxide	CO ₂	.017
hydrogen radical	H	.010
hydrogen	H ₂	.020
water vapor	H ₂ O	.114
nitric oxide	NO	.004
nitrogen	N ₂	.109
hydroxide	OH	.018
oxygen	O ₂	.032
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.656
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 38.07 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 17OXIDIZER/FUEL MOLE RATIO 7.00PERCENT MIXING 80VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 4.78
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$ 0

RESULTS:Flame Temperature 674 °K (1214 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.024
carbon dioxide	CO ₂	.020
hydrogen radical	H	.011
hydrogen	H ₂	.023
water vapor	H ₂ O	.132
nitric oxide	NO	.005
nitrogen	N ₂	.125
hydroxide	OH	.021
oxygen	O ₂	.037
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.603
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 36.91 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 18OXIDIZER/FUEL MOLE RATIO 7.00PERCENT MIXING 60VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 3.59
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$ 0

RESULTS:Flame Temperature 920 °K (1657 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.028
carbon dioxide	CO ₂	.023
hydrogen radical	H	.013
hydrogen	H ₂	.027
water vapor	H ₂ O	.155
nitric oxide	NO	.005
nitrogen	N ₂	.147
hydroxide	OH	.024
oxygen	O ₂	.044
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.533
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 35.25 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 19OXIDIZER/FUEL MOLE RATIO 7.00PERCENT MIXING 40VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} = \underline{0}$ $a_{14} = \underline{0}$ $a_{15} = \underline{2.39}$
 $a_{16} = \underline{0}$ $a_{17} = \underline{0}$ $a_{18} = \underline{0}$
 $a_{19} = \underline{0}$

RESULTS:Flame Temperature 1267 °K (2281 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.034
carbon dioxide	CO ₂	.028
hydrogen radical	H	.016
hydrogen	H ₂	.032
water vapor	H ₂ O	.189
nitric oxide	NO	.007
nitrogen	N ₂	.179
hydroxide	OH	.030
oxygen	O ₂	.053
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.432
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 32.97 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 20OXIDIZER/FUEL MOLE RATIO 7.00PERCENT MIXING 20VAPORIZATION CONDITIONS Excess N_2O_4 (l) 100% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 1.20
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$ 0

RESULTS:Flame Temperature 1840 °K (3313 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.044
carbon dioxide	CO ₂	.036
hydrogen radical	H	.020
hydrogen	H ₂	.041
water vapor	H ₂ O	.240
nitric oxide	NO	.008
nitrogen	N ₂	.228
hydroxide	OH	.038
oxygen	O ₂	.068
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.276
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.000

Average Molecular Weight 29.38 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 21OXIDIZER/FUEL MOLE RATIO 8.549PERCENT MIXING 100VAPORIZATION CONDITIONS Excess N_2O_4 (l) 88% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 6.59
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$.93

RESULTS:Flame Temperature 361 °K (650 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.019
carbon dioxide	CO ₂	.015
hydrogen radical	H	.009
hydrogen	H ₂	.017
water vapor	H ₂ O	.102
nitric oxide	NO	.004
nitrogen	N ₂	.097
hydroxide	OH	.016
oxygen	O ₂	.029
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.646
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.046

Average Molecular Weight 41.06 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 22OXIDIZER/FUEL MOLE RATIO 13.02PERCENT MIXING 100VAPORIZATION CONDITIONS Excess N_2O_4 (l) 40% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} =$ 0 $a_{14} =$ 0 $a_{15} =$ 4.84
 $a_{16} =$ 0 $a_{17} =$ 0 $a_{18} =$ 0
 $a_{19} =$ 7.16

RESULTS:Flame Temperature 319 °K (575 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.016
carbon dioxide	CO ₂	.014
hydrogen radical	H	.008
hydrogen	H ₂	.015
water vapor	H ₂ O	.090
nitric oxide	NO	.003
nitrogen	N ₂	.086
hydroxide	OH	.014
oxygen	O ₂	.026
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.418
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.310

Average Molecular Weight 54.04 lbs/lb-mole

THERMOCHEMICAL DATA SHEET

ANALYSIS NO. 23

OXIDIZER/FUEL MOLE RATIO 17.72

PERCENT MIXING 100

VAPORIZATION CONDITIONS Excess N_2O_4 (l) 18% Dissociated into NO_2 (g)

COEFFICIENTS FOR UNREACTED PROPELLANT SPECIES:

$a_{13} = $ <u>0</u>	$a_{14} = $ <u>0</u>	$a_{15} = $ <u>2.97</u>
$a_{16} = $ <u>0</u>	$a_{17} = $ <u>0</u>	$a_{18} = $ <u>0</u>
$a_{19} = $ <u>13.73</u>		

RESULTS:

Flame Temperature 296 °K (533 °R)

<u>Fireball Species</u>	<u>Formula</u>	<u>Mole Fraction</u>
carbon monoxide	CO	.015
carbon dioxide	CO ₂	.012
hydrogen radical	H	.007
hydrogen	H ₂	.014
water vapor	H ₂ O	.080
nitric oxide	NO	.003
nitrogen	N ₂	.076
hydroxide	OH	.013
oxygen	O ₂	.023
hydrazine vapor	N ₂ H ₄ (g)	.000
UDMH vapor	C ₂ H ₈ N ₂ (g)	.000
nitrogen dioxide	NO ₂	.229
ammonia	NH ₃ (g)	.000
nitrogen tetroxide	N ₂ O ₄ (g)	.529

Average Molecular Weight 64.80 lbs/lb-mole

APPENDIX C
COMPUTER OUTPUT, REACTIONS OF LIQUID ROCKET PROPELLANTS
WITH OTHER CHEMICALS

Case No.	Oxidant	Fuel	Page
34	Nitrogen Tetroxide	Methylene Chloride	111
35	Nitrogen Tetroxide	Ethlene Glycol	112
36	Nitrogen Tetroxide	Dichloroethane	113
37	Nitrogen Tetroxide	Liquid Propane	114
38	Nitrogen Tetroxide	Octane	115
39	Nitrogen Tetroxide	Acetone	116
40	Nitrogen Tetroxide	Acetylene	117
41	Nitrogen Tetroxide	Amonia	118
42	LOX	Aerozine-50	119
43	Air	Aerozine-50	120
44	Chlorine	Aerozine-50	121
45	Nitric Acid	Aerozine-50	122
46	Hydrogen Peroxide	Aerozine-50	123

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 34

CHEMICAL FORMULA

OXIDANT N 2.00000 O 4.00000
FUEL C 1.00000 H 2.00000 CL 2.00000

WT FRACTION (SEE NOTE)
1.00000 1.00000 1.00000
STATE L L L
TEMP DEG K 298.15 298.15 298.15
DENSITY G/CC 0.0000 0.0000 0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= .6393 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.0000
T. DEG K 2325
H. CAL/G -190.2
S. CAL/(G)(K) 1.9486
M. MOL WT 34.423
(DLV/DLP)T -1.00839
(DLV/DLP)P 1.1775
CP. CAL/(G)(K) .5299
GAMMA (S) 1.1664
CPF. CAL/(G)(K) .2828
SON VEL. M/SEC 809.3

MOLE FRACTIONS

CO .00704
CO2 .19561
CL .11539
CLO .00053
CL2 .00292
H .00021
HCL .28355
H2 .00037
H2O .05769
NO .00682
NO2 .00001
N2 .18365
O .00212
OH .00540
O2 .13870

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CCL	CCL2	CCL3	CCL4	CH	CH2	CH2O	CH3
CH4	CN	CNN	CN2	COCL	COCL2	C2	C2CL2	C2H	C2H2
C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2	C4
C5	CLCN	CLO2	CL2O	HCN	HCO	HNC	HNO	HNO2	HNO3
H2O	H2O(S)	H2O(L)	H2O2	N	NC	NH	NH2	NH3	NOCL
NO2CL	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 35
 CHEMICAL FORMULA
 OXIDANT N 2.00000 O 4.00000
 FUEL C 2.00000 H 6.00000 O 2.00000
 O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 1.4899 DENSITY= 0.0000
 WT FRACTION (SEE NOTE) 1.00000 -4676.000 L 298.15 0.0000
 1.00000 -108560.000 L 298.15 0.0000

THERMODYNAMIC PROPERTIES

P, ATM 1.000
 T, DEG K 2215
 H, CAL/G -900.1
 S, CAL/(G)(K) 2.9664
 M, MOL WT 21.840
 (DLV/DLP)T -1.00083
 (DLV/DLT)P 1.0219
 CP, CAL/(G)(K) .5497
 GAMMA (S) 1.2078
 CPF, CAL/(G)(K) .4888
 SON VEL, M/SEC 1009.2

MOLE FRACTIONS

CO .24468
 CO2 .10719
 H .00243
 H2 .15950
 H2O .36670
 NO .00003
 N2 .11867
 O .00001
 OH .00079
 O2 .00001

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNH	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	HNC	HNO	HNO2	HNO3
H2O	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO2
N2	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O3	

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 36

CHEMICAL FORMULA

OXIDANT N 2.00000 O 4.00000
FUEL C 2.00000 H 4.00000 CL 2.00000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 1.1316 DENSITY= 0.0000

WT FRACTION (SEE NOTE) 1.00000 1.00000
ENTHALPY CAL/MOL -4676.000 -39700.000
STATE L L
TEMP DEG K 298.15 298.15
DENSITY G/CC 0.0000 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2744
H. CAL/G -226.0
S. CAL/(G)(K) 2.2532
M. MOL WT 30.337
(DLV/DLP)T -1.02720
(DLV/DLT)P 1.6036
CP. CAL/(G)(K) 1.2256
GAMMA (S) 1.1239
CPF. CAL/(G)(K) -3314
SON VEL. M/SEC 919.4

MOLE FRACTIONS

CO .15673
CO2 .14982
CL .07058
CLO .00008
CL2 .00014
H .01025
HCL .23560
H2 .02369
H2O .15121
NO .00397
N2 .16287
O .00486
OH .01745
O2 .01273

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CCL	CCL2	CCL3	CCL4	CH	CH2	CH2O	CH3
CH4	CN	CNN	CN2	COCL	COCL2	C2	C2CL2	C2H	C2H2
C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3	C3O2	C4
C5	CLCN	CLO2	CL2O	HCN	HCO	HACO	HNO	HNO2	HNO3
H02	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NOCL
NO2	NO2CL	NO2	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

CASE NO. 37

CHEMICAL FORMULA

CHEMICAL FORMULA	
OXIDANT N	2.00000 0 4.00000
FUEL C	3.00000 H 8.00000

WT FRACTION (SEE NOTE)	ENTHALPY CAL/MOL	STATE	TEMP DEG K	DENSITY G/CC
1.00000	-4676.000	L	298.15	0.0000
1.00000	-30372.000	L	231.00	0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 5.2164 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM	1.000
T. DEG K	1013
H. CAL/G	-369.8
S. CAL/(G)(K)	3.3318
MOL WT	15.142
(DLV/DLP)T	-1.06793
(DLV/DLT)P	2.0262
CP. CAL/(G)(K)	2.7647
GAMMA (S)	1.1454
CEPF, CAL/(G)(K)	.6056
SON VEL/M/SEC	798.2

MOLE FRACTIONS

C(S)	.18445
CH4	.02359
CO	.19196
CO2	.02006
H2	.47646
H2O	.03635
NH3	.00006
N2	.06708

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

[illegible]

NOTE: WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 38

CHEMICAL FORMULA
OXIDANT N 2.00000 O 4.00000
FUEL C 8.00000 H 18.00000

WT FRACTION (SEE NOTE)
1.00000
1.00000
ENTHALPY CAL/MOL
-4676.000
-59740.000
STATE L L
TEMP DEG K
298.15
298.15
DENSITY G/CC
0.0000
0.0000

EQUIVALENCE RATIO= 5.0342 DENSITY= 0.0000

PERCENT FUEL= 50.0000

O/F= 1.0000

THERMODYNAMIC PROPERTIES

P, ATM 1.000
T, DEG K 1057
H, CAL/G -286.9
S, CAL/(G)(K) 3.2004
M, MOL WT 15.922
(DLV/DLP)T -1.04810
(DLV/DLP)P 1.7106
CP, CAL/(G)(K) 1.9567
GAMMA (S) 1.1608
CPF, CAL/(G)(K) .5728
SON VEL, M/SEC 800.6

MOLE FRACTIONS

C(S) .19137
CH4 .01398
CO .23277
CO2 .01271
H2 .45751
H2O .02166
NH3 .00004
N2 .06994

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C	CH	CH2	CH2O	CH3	CN	CNN	CN2	C2H
C2H2	C2H4	C2H6	C2N	C2N2	C2N2H8(L)	C2N2H8	C2O	C3O2
C4	C5	H	HCN	HCO	HNC	HNO	HNO2	HO2
H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO3
N2H4	N2H4(L)	N2O	N2O4	N2O5	N3	N3	O	O2
O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 39

CHEMICAL FORMULA

OXIDANT N 2.00000 O 4.00000
FUEL C 3.00000 H 6.00000 O 1.00000

D/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.5532 DENSITY= 0.0000

WT FRACTION ENTHALPY STATE TEMP DENSITY
(SEE NOTE) CAL/MOL DEG K G/CC
1.00000 -4676.000 L 298.15 0.0000
1.00000 -59320.000 L 298.15 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 1276
H. CAL/G -536.1
S. CAL/(G)(K) 3.0759
M. MOL WT 17.520
(DLV/DLP)T -1.00025
(DLV/DLP)P 1.0028
CP. CAL/(G)(K) .4899
GAMMA (S) 1.3031
CPF. CAL/(G)(K) .4684
SON VEL. M/SEC 888.4

MOLE FRACTIONS

CH4 .00006
CO .42175
CO2 .03066
H2 .40375
H2O .04858
NH3 .00001
N2 .09520

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CN	CNM	CN2	C2
C2H	C2H2	C2H4	C2H6	C2N	C2H2	C2N2H8(L)	C2N2H8	C2O	C3
C3O2	C4	C5	H	HCN	HCO	HNC	HNO	HNO2	HNO3
H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NO	NO2
NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O	OH
O2	O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 40

CHEMICAL FORMULA

OXIDANT N 2.00000 O 4.00000
FUEL C 2.00000 H 2.00000

O/F = 1.0000 PERCENT FUEL = 50.0000 EQUIVALENCE RATIO = 4.4171 DENSITY = 0.0000

WT FRACTION
(SEE NOTE)
1.00000
1.00000

ENTHALPY
CAL/MOL

-4676.000
49270.000

STATE
L
L

TEMP
DEG K

298.15
192.50

DENSITY
G/CC

0.0000
0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2895
H. CAL/G 920.7
S. CAL/(G)(K) 3.0852
M. MOL WT 20.797
(DLV/DLP)T -1.01737
(DLV/DLT)P 1.3508
CP. CAL/(G)(K) 1.4472
GA**MA (S) 1.1150
CPF. CAL/(G)(K) .5115
SON VEL. M/SEC 1135.9

MOLE FRACTIONS

C(S) .21193
C .00002
CH .00001
CH2 .00001
CH3 .00003
CH4 .00001
CN .00053
CO .35624
C2 .00001
C2H .00437
C2H2 .01388
C2N .00013
C2N2 .00004
C3 .00007
H .05092
HCN .02359
H2 .26132
N2 .07689

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

CH2O	CNN	CO2	C2H4	C2H6	C2N2H8(L)	C2N2H8	C2O	C3O2
C4	C5	H2CO	H2O	H2O2	H2O3	H2O	H2O(S)	H2O(L)
H2O	H2O2	N	NH	NH2	NH3	N2	N2O	N2O3
N2H4	N2H4(L)	N2O	N2O4	N2O5	N3	O	OH	O2
O3								

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 41

CHEMICAL FORMULA

OXIDANT N 2.00000 O 4.00000
FUEL N 1.00000 H 3.00000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.0260 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 1674
H. CAL/G -525.4
S. CAL/(G)(K) 3.6209
M. MOL WT 15.588
(DLV/DLP)T -1.00002
(DLV/DLT)P 1.0006
CP. CAL/(G)(K) .6003
GAMMA (S) 1.2700
CPF. CAL/(G)(K) .5979
SON VEL. M/SEC 1064.8

MOLE FRACTIONS

H .00007
H2 .34759
H2O .33882
N2 .31352

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

HNO	HNO2	HNO3	H2O	H2O(S)	H2O(L)	H2O2	N	NH	NH2
NH3	NO	NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5
N3	O	OH	O2	O3					

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 42

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT O 2.00000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 1.5841 DENSITY= 0.0000

WT FRACTION (SEE NOTE)
.50000
.50000
1.00000

STATE

ENTHALPY
CAL/MOL

TEMP
DEG K

DENSITY
G/CC

12100.000 L 298.15 0.0000
11900.000 L 298.15 0.0000
-3102.000 L 90.18 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 2923
M. CAL/G 95.4
S. CAL/(G)(K) 3.5798
M. MOL WT 18.045
(DLV/DLP)T -1.02928
(DLV/DLP)P 1.6086
CP CAL/(G)(K) 1.9817
GAMMA (S) 1.1293
P. CAL/(G)(K) 5703
SON VEL./M/SEC 1233.2

MOLE FRACTIONS

CO .12091
CO2 .02921
H .05493
H2 .19955
H2O .34012
NO .00304
N2 .21431
O .00508
OH .02932
O2 .00351

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S) C C2H C2H2 CH CH2 CH2O CH3 CH4 CN C2H2+H8(L) CHN C2H C2O
C2 C2H C302 C4 C5 H2O(L) H2O4(L) N2O4(L) N2O5
C3 C302 H2O(S) N2H4(L) N2O HCN NCO NH NH2 NH3 NO2
NO3 N2H4

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 43

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000
OXIDANT N 1.56176 O .41959 AR .00932 C .00030

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 6.7500 DENSITY= 0.0000

WT FRACTION (SEE NOTE)
ENTHALPY CAL/MOL
STATE
TEMP DEG K
DENSITY G/CC

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 1072
H. CAL/G 143.4
S. CAL/(G)(K) 3.2190
M. MOL WT 15.653
(DLV/DLP)T -1.01687
(DLV/DLP)P 1.2123
CP. CAL/(G)(K) .8596
GAMMA (S) 1.2503
CPF. CAL/(G)(K) .4997
SON VEL. M/SEC 843.9

MOLE FRACTIONS

AP .00248
C(S) .01420
CH4 .01048
CO .10224
CO2 .00154
HCN .00001
H2 .46998
H2O .00646
NH3 .00008
N2 .39254

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C CH CH2 CH2O CH3 C2H2 C2H4 C2H6 C2H8 C2H10
C2H2 C2H4 C2H6 C2H8 C2H10
C4 C5 C6 C7 C8 C9 C10 C11 C12 C13
H2O(L) H2O2 N2O N2O4 N2O6 N2O8 N2O10 N2O12 N2O14 N2O16
N2H4(L) N2H4(N) N2H4(S) N2H4(L) N2H4(N) N2H4(S)

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 44

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT CL 2.00000

WT FRACTION (SEE NOTE)
.50000
.50000
1.00000

ENTHALPY CAL/MOL
12100.000
11900.000
-5391.000

STATE
L
L
L

TEMP DEG K
298.15
298.15
239.09

DENSITY G/CC
0.0000
0.0000
0.0000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 6.9319 DENSITY= 0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.0000
T. DEG K 1318
M. CAL/G 109.9
S. CAL/(G)(K) 2.6769

M. MOL WT 19.543
(DLV/DLP)T -1.00166
(DLV/DLP)P 1.0139
CP. CAL/(G)(K) .4587
GAMMA (S) 1.2924
CPF. CAL/(G)(K) .4455
SON VEL. M/SEC 851.2

MOLE FRACTIONS

C(S) .13856
CH4 .00143
HCL .23743
HCN .00007
H2 .42117
N2 .00002
N2 .20133

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN 10^-6 FOR ALL ASSIGNED CONDITIONS

C CCL CCL2 CCL3 CCL4 CH C2H2 C2H4 CH3 CN C2N2H8(L) N2
C2H2 C2 C2CL2 C2H C2H2 C2H4 CLCN C2N C2N2 N4
N2H2 N2H4 N2H4(L) N3

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 45

CHEMICAL FORMULA

	FUEL	OXIDANT	N	H	O	PERCENT FUEL	EQUIVALENCE RATIO	DENSITY
FUEL	2.00000	4.00000	2.00000	8.00000	0.00000	50.0000	2.2201	0.0000
OXIDANT	1.00000	1.00000	1.00000	0.00000	0.00000			

WT FRACTION (SEE NOTE)

ENTHALPY CAL/MOL

STATE

TEMP DEG K

DENSITY G/CC

THERMODYNAMIC PROPERTIES

P. ATM 1.000

T. DEG K 2123

H. CAL/G -185.1

S. CAL/(G)(K) 3.5836

M. MOL WT 16.521

D.V/DLP)T -1.00058

(DLV/DLT)P 1.0152

CP. CAL/(G)(K) .6272

GAMMA (S) 1.2455

GPF CAL/(G)(K) .5755

SON VEL.M/SEC 1153.5

MULE FRACTIONS

CO .12108

CO2 .01637

H .00213

H2 .35779

H2O .23929

NO .00001

N2 .26316

OH .00017

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2H	CH3	CH4	CN	CNH	CN2
C2	C2H	C2H2	C2H4	C2H6	C2H8	C2H10	C2H12	C2H14	C2H16
C3	C3H	C3H2	C3H4	C3H6	C3H8	C3H10	C3H12	C3H14	C3H16
H2	H2O(S)	H2O(L)	H2O2	N	N2O	N2O2	N2O4	N2O6	N2O8
NO3	N2H4	N2H4(L)	N2H4(L)	N2H4(L)	N2H4(L)	N2H4(L)	N2H4(L)	N2H4(L)	N2H4(L)
O3									

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS

THEORETICAL THERMODYNAMIC COMBUSTION PROPERTIES

CASE NO. 46

CHEMICAL FORMULA

FUEL N 2.00000 H 4.00000
FUEL C 2.00000 H 8.00000 N 2.00000
OXIDANT H 2.00000 O 2.00000

O/F= 1.0000 PERCENT FUEL= 50.0000 EQUIVALENCE RATIO= 2.1627 DENSITY= 0.0000

WT FRACTION (SEE NOTE)
.50000
.50000
1.00000
ENTHALPY CAL/MOL
12100.000
11900.000
-44860.000
STATE
L
L
L
TEMP DEG K
298.15
298.15
298.15
DENSITY G/CC
0.0000
0.0000
0.0000

THERMODYNAMIC PROPERTIES

P. ATM 1.000
T. DEG K 1939
M. CAL/G -515.5
S. CAL/(G)(K) 3.8849
M. MOL WT 14.871
(DLV/DLP)T -1.00019
(DLV/DLP)P 1.0051
CP. CAL/(G)(K) .6665
GAMMA (S) 1.2537
CPF. CAL/(G)(K) .6419
SON VEL. M/SEC 1165.9

MOLF. FRACTIONS

CO .10569
CO2 .01803
H .00067
H2 .40230
H2O .29539
N2 .17787
OH .00004

ADDITIONAL PRODUCTS WHICH WERE CONSIDERED BUT WHOSE MOLE FRACTIONS WERE LESS THAN .000005 FOR ALL ASSIGNED CONDITIONS

C(S)	C	CH	CH2	CH2O	CH3	CH4	CN	CNH	CN2
C2	C2H	C2H2	C2H4	C2H6	C2N	C2H2	C2H2H8(L)	C2H2H8	C2O
C3	C3O2	C4	C5	HCN	HCO	H2CO	H4O	H4O2	H4O3
H2	H2O(S)	H2O(L)	H2O2	N	NCO	NH	NH2	NH3	NO
NO2	NO3	N2H4	N2H4(L)	N2O	N2O4	N2O4(L)	N2O5	N3	O
O2	O3								

NOTE. WEIGHT FRACTION OF FUEL IN TOTAL FUELS AND OF OXIDANT IN TOTAL OXIDANTS